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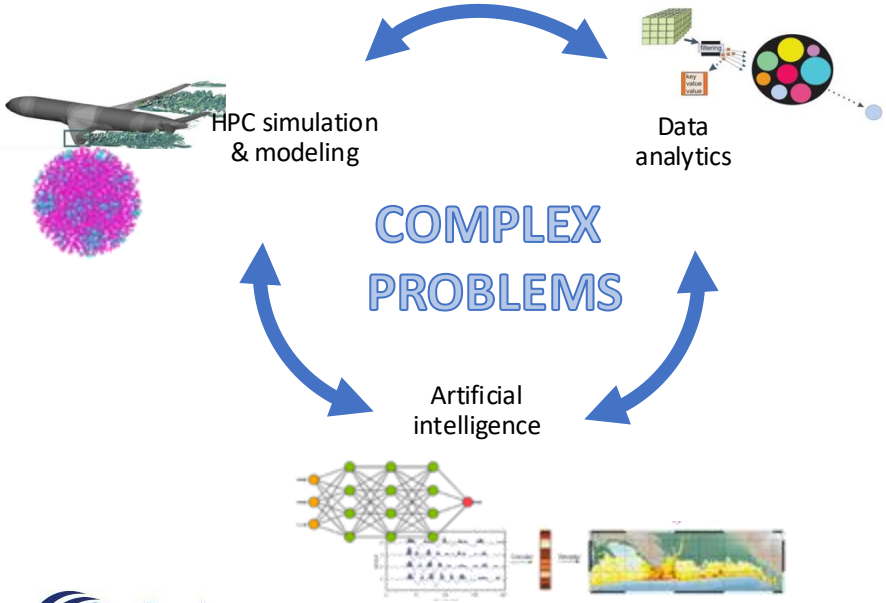
CONNECTING THE DOTS
ISC High Performance

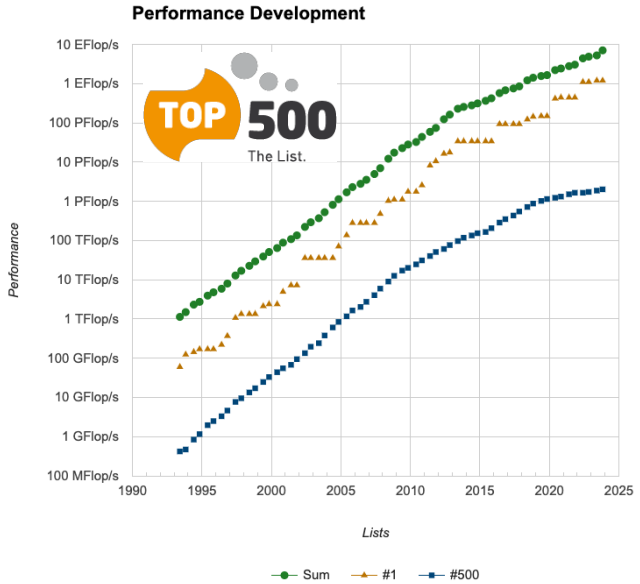
COMPSs: Task-based Approach to Autonomous Laboratories

Rosa M Badia, BSC

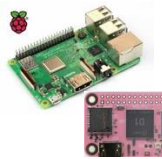
1st Advancing Autonomous Scientific Discovery Workshop

Complex problems for complex computing infrastructures





Digital continuum



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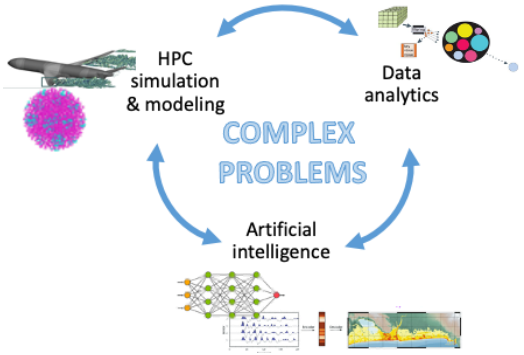
Workflow lifecyle challenges

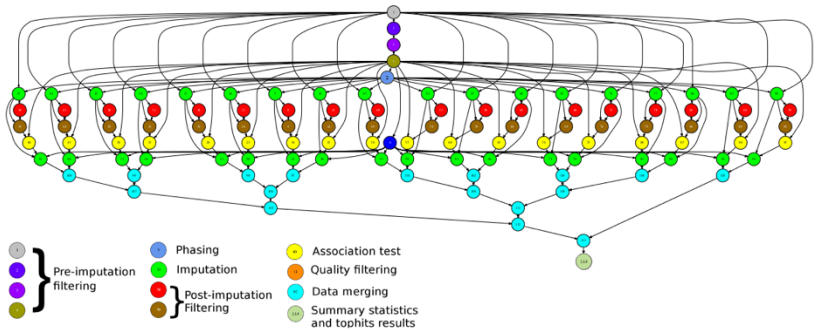


- Workflow development
  - Different programming models and environments
- Workflow deployment
  - Can we make it easier to new HPC users?
- Workflow operation
  - Go beyond static workflows
  - Not only computational aspects, data management as well

Workflows in PyCOMPSs

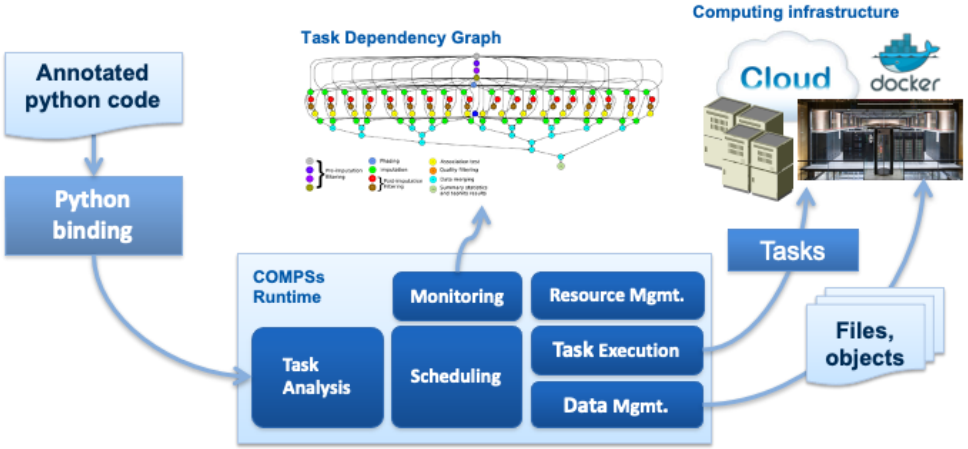
- Sequential programming, parallel execution
  - General purpose programming language + annotations/hints
- Task-based parallelization
  - Automatic generation of task graph
  - Coarse grain tasks: methods and web services
  - Sequential and parallel tasks
- Offers a shared memory illusion in a distributed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

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



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

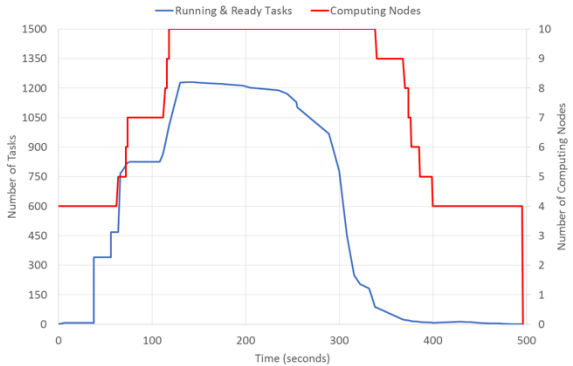


Some features towards autonomous execution

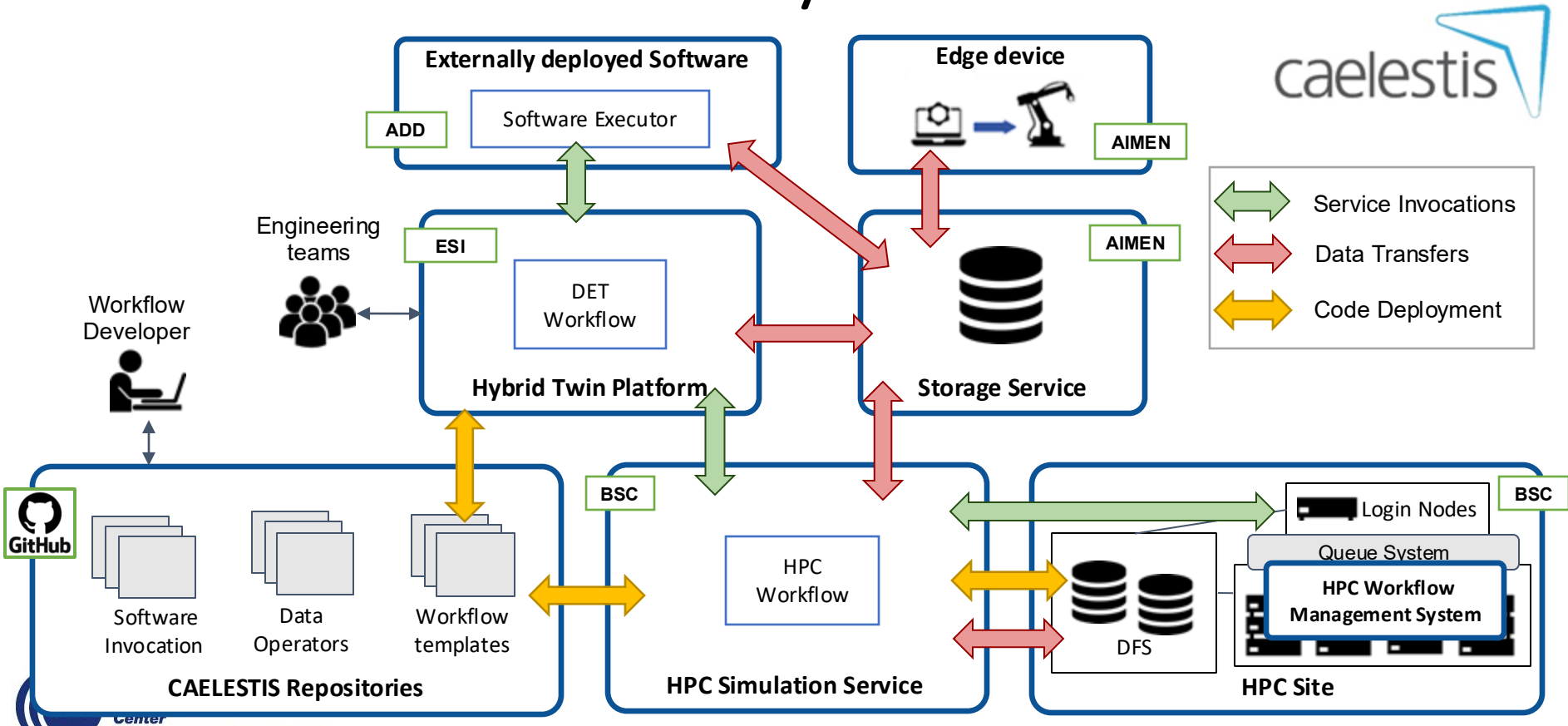
- Fault tolerance
- Time outs
- Exceptions
- Task constraints
- Elasticity
- Checkpointing

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

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

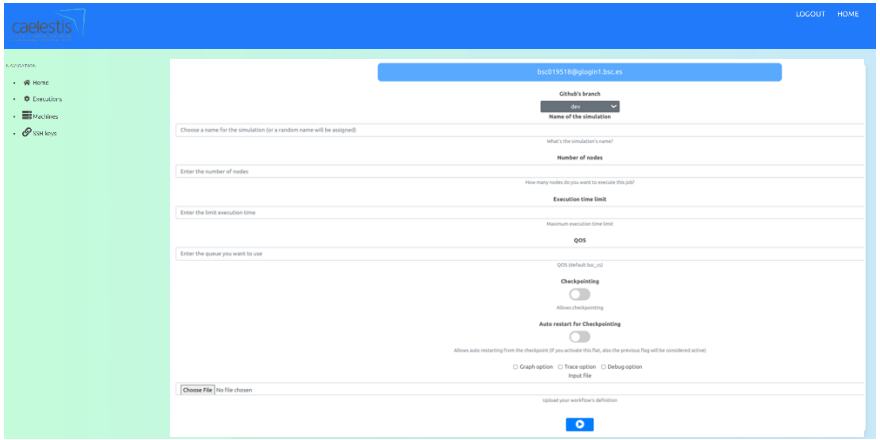


CAELESTIS Simulation Ecosystem Architecture



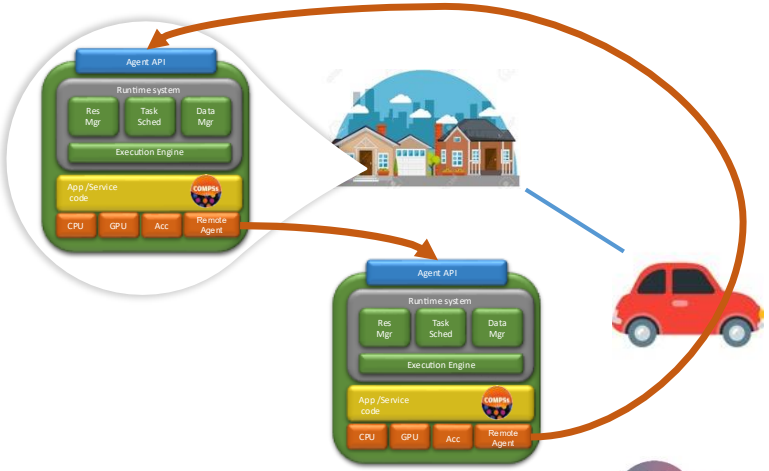
CAELESTIS Simulation service

- Web interface for the support of workflow management in CAELESTIS
- Two management options of checkpointed jobs:
  - **Manual handling**: users have the option to handle checkpoints manually. If a job ends due to a time constraint, it will appear in the execution dashboard under the ”timeout jobs” list. Users can then initiate a new job from the checkpoint.
  - **Automatic handling**: If job terminates due to time constraint, the service reinitiates the workflow submission, which is rerun from the checkpoint. This process can continue until the job concludes successfully.



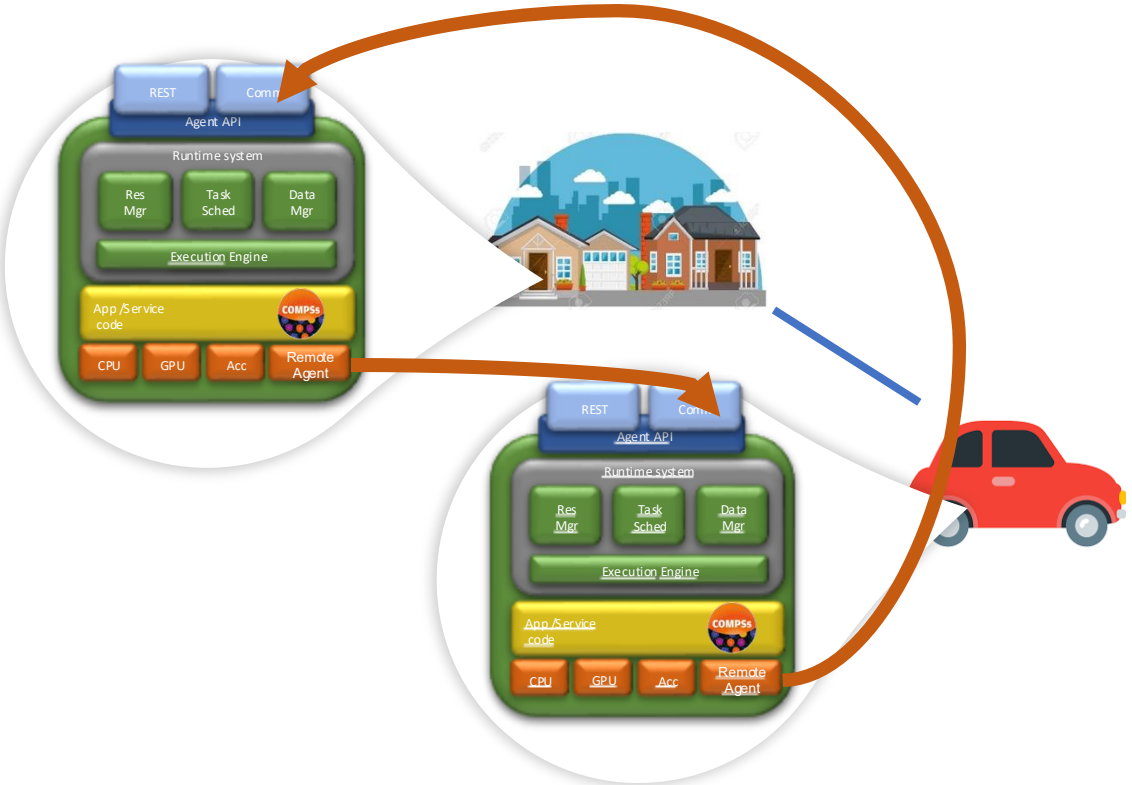
COMPSs Agents for the edge-to-cloud continuum

- **Decentralized** approach to deal with large amounts of data and unstable infrastructures
- COMPSs agents: new organization of the COMPSs runtime to handle distribution, parallelism and heterogeneity
- Runtime deployed as a standalone agent:
  - Can run application logic
  - Can detect parallelism within application logic
  - Can interact with other agents, offloading tasks to peers
- Malleable organization
  - Hierarchical but dynamic structure
  - Support for nesting
- Edge-to-Edge and edge-to-cloud



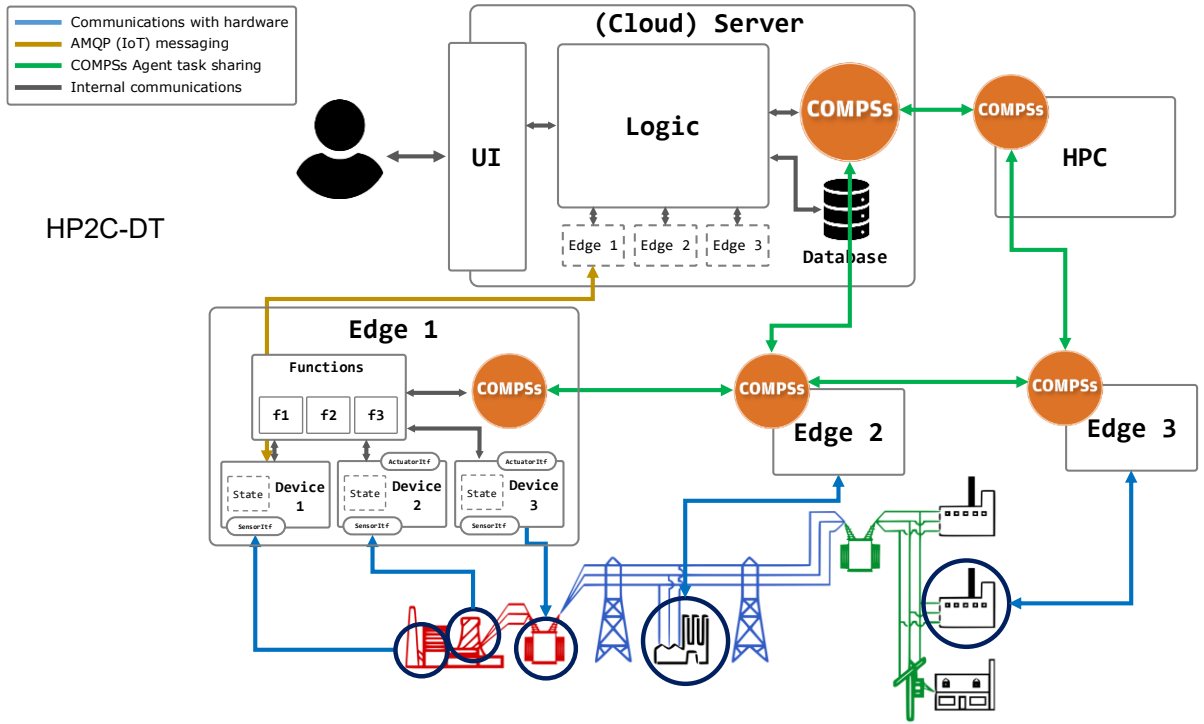
COMPSs Agents interaction

- One agent in each node of the continuum
- Offers a service interface that receives compute requests
- The agent registers the execution request and submits it to the runtime
- Agents can offload computation onto other agents by adding them onto their resource pool



HP2C-DT: a digital twin for renewable electrical networks

- User Interface supports monitoring and visualization of network status
- Submission of HPC COMPSs jobs from UI
- COMPSs agents deployed in edge devices
- A Device can be a Sensor, an Actuator, or both
- Sensors make measurements available to the Digital Twin and can trigger functions



COLMENA: swarm oriented continuum

- COLMENA programming model
  - Service oriented
  - Services defined as a set of distributed roles
  - Each role defines the required properties of the hosting device
    - i.e., @Requirements("/devices/camera")
- COLMENA agents
  - Decentralized orchestration with autonomous agents
  - Cooperative roles played by the devices
  - Devices decide their role based on capabilities and context
  - Metrics monitoring to meet the KPIs
    - i.e., @KPI("processing_time < 3s")
  - Dynamic adaptability
    - Devices can start/stop playing a role

Project in early stages, demonstration prototype

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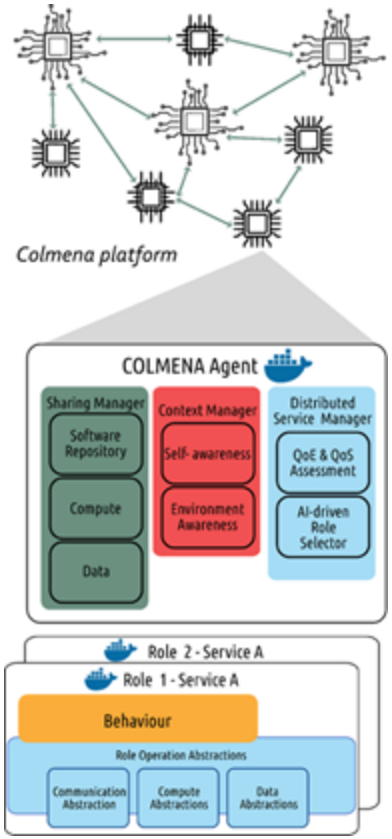
Colmena

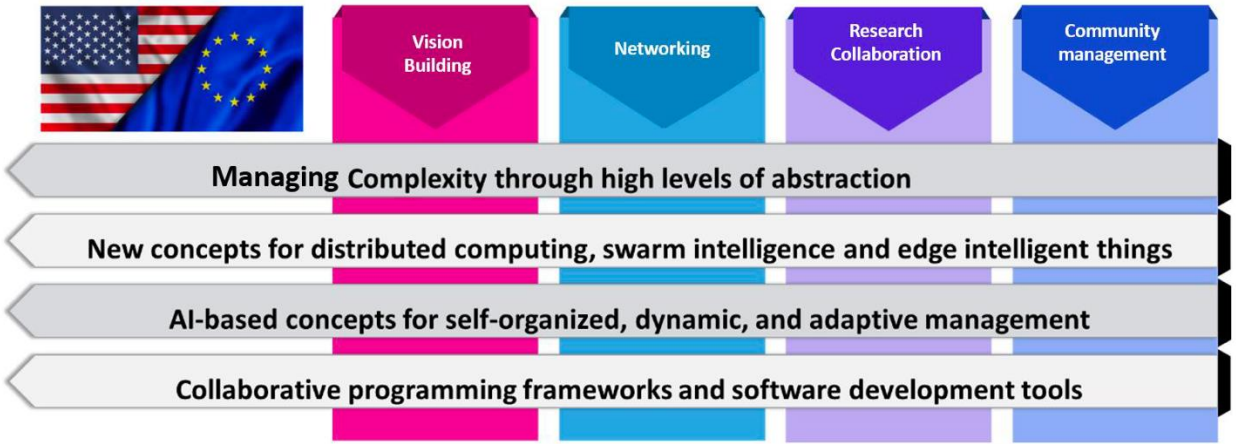
COLMENA platform

- Each device in the platform hosts an Agent
- Three main components:
  - Sharing Manager
    - Supports interaction with the platform to publish software, share data and operate on it across the continuum
  - Context Manager
    - Provides Agents awareness of their **self-context** – capacities, identity, location and ownership
    - and **social context** – neighbouring devices capabilities, proximity, volatility and trustworthiness
  - Distributed Service Manager
    - Selects roles to be hosted locally to contribute to the overall service performance
    - QoE & QoS Assessment
    - AI model that determines the number of instances of each role to be played by the device



DISCOVER US

- Strengthen long-term collaboration between the EU and the US on new concepts and visions for the computing continuum, distributed computing and swarm intelligence.
  - By creating networking and collaboration opportunities to promote cooperation
- Organization of networking events, exchange and fellowship programs, training
- 66 members from 18 countries
- First call for exchanges funded
  - 7 exchanges funded
- Second call under evaluation
- Next call in October 2025
- Vision paper



Key research topics

Project duration: 30 months
Involve 100 senior researchers funding 20 pre-competitive transatlantic research collaborations.

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Further Information

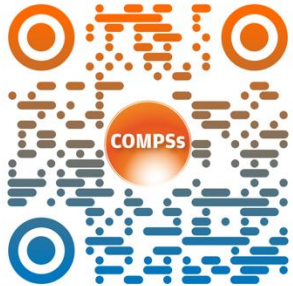
- Project page: http://www.bsc.es/compss
  - Documentation
  - Virtual Appliance for testing & sample applications
  - Tutorials
- Source Code

  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/



ACKs

HP2C-DT

CAELESTIS

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Thanks!

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