OpenMOLE: a grid enabled workflow platform

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Introduction

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- design of experiments,
- genetic algorithms,
- stochastic simulations with many replications,
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=> It is possible to develop a **generic software framework** for distributing naturally parallel application.

Outline

1. Genesis of OpenMOLE
2. Central concepts
3. Task delegation
4. Detailed example
5. Scientific projects

From a sequential approach...

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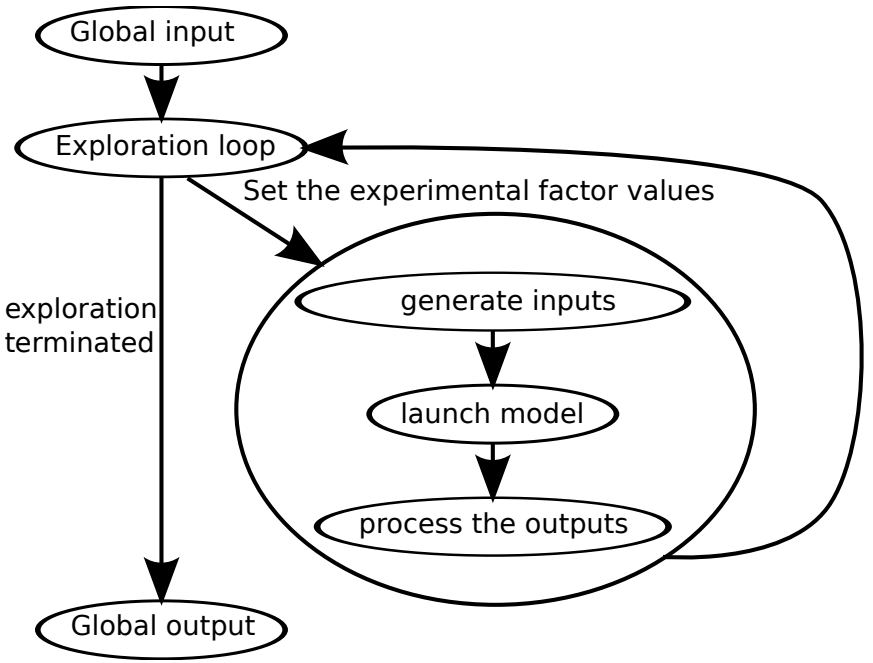

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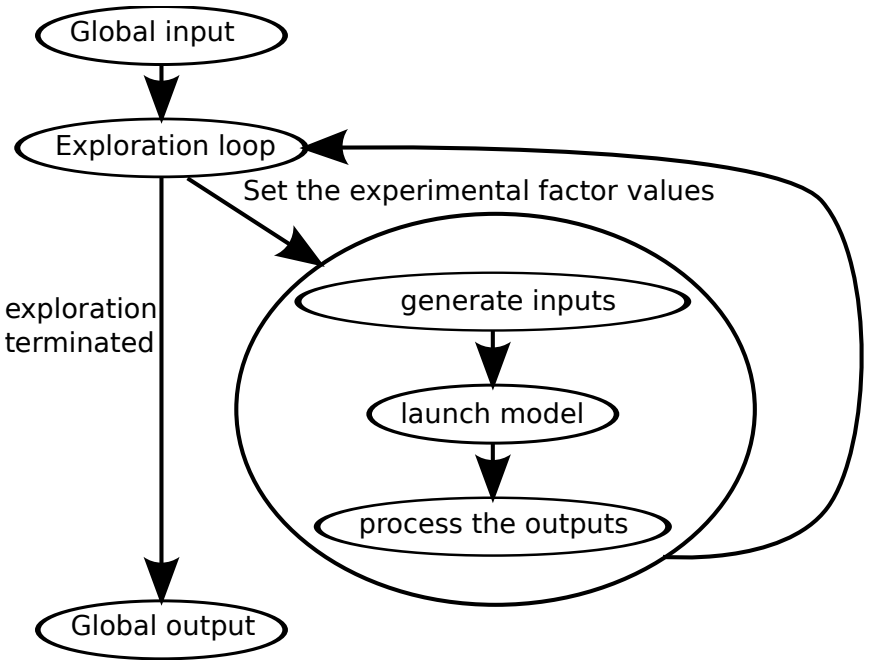

These concepts were inherently **sequential !**

... to a distributed approach.

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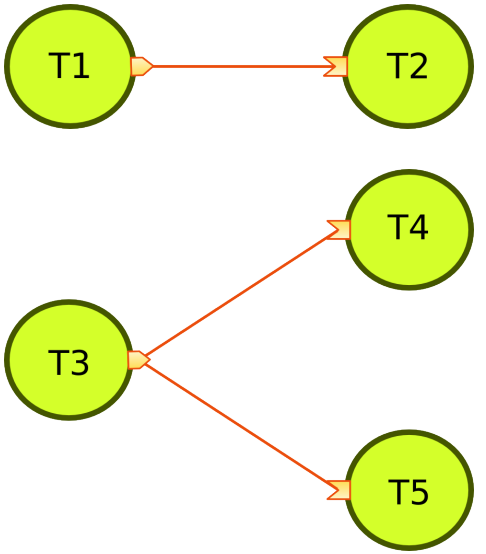

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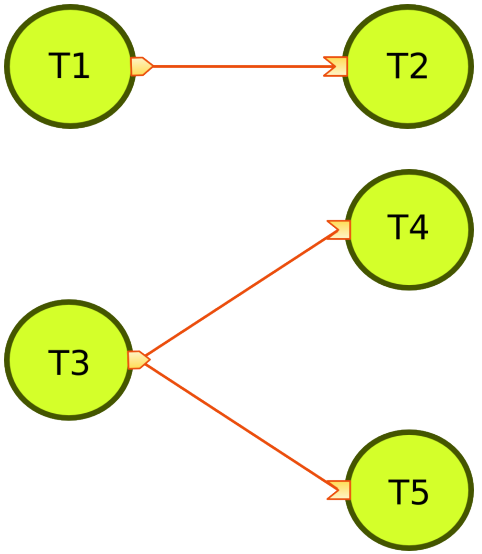

Untie distributed algorithms and execution environments = environment agnostic distributed algorithms.

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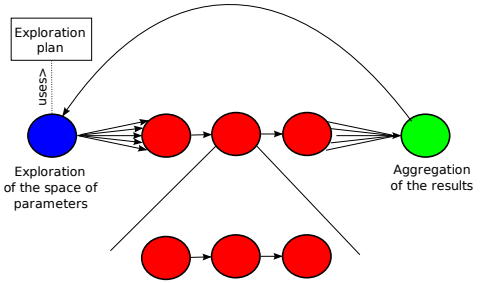
OpenMOLE:

- allows **the definition of complex workflows** for model exploration,



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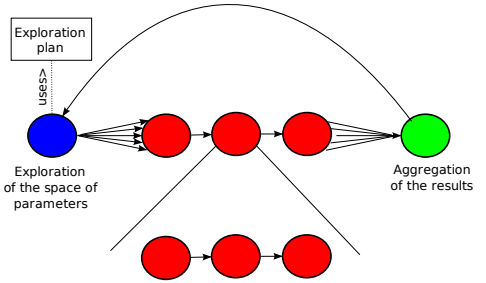

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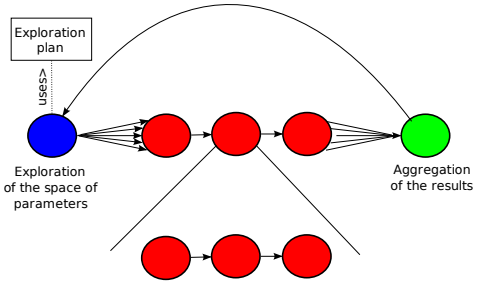
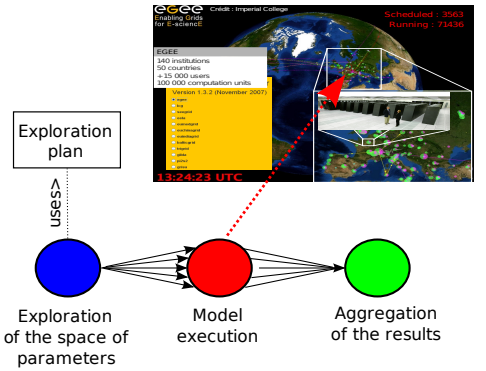


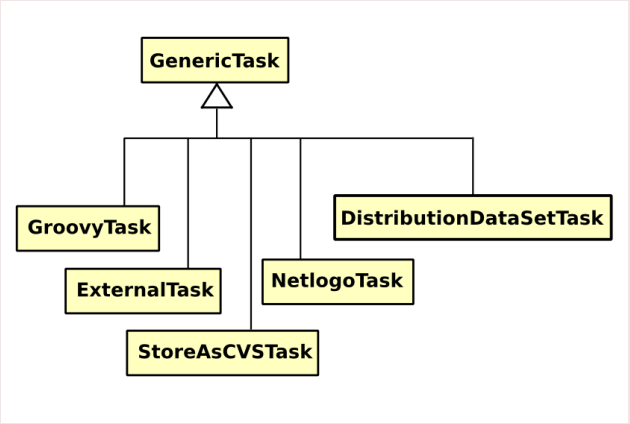
- **manages the execution** of these workflows on the user desktop PC,

- provides **transparent delegation mechanisms** of part of these workflow's execution **to distributed environments** (grids, clusters, ssh servers).



Tasks

Definition



A Task is a polymorphic class that embed a work to be achieved. Tasks are portable and can be executed on any execution environment.

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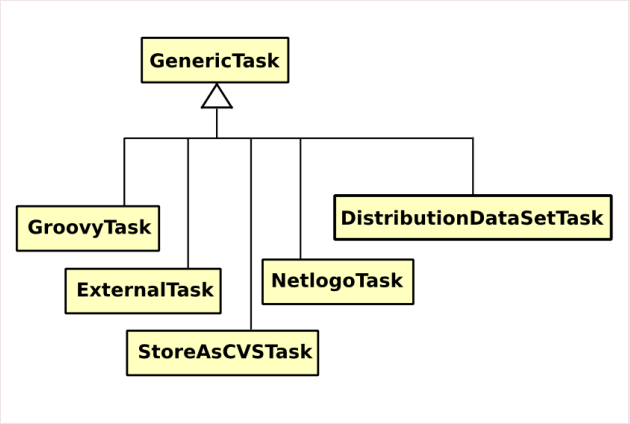

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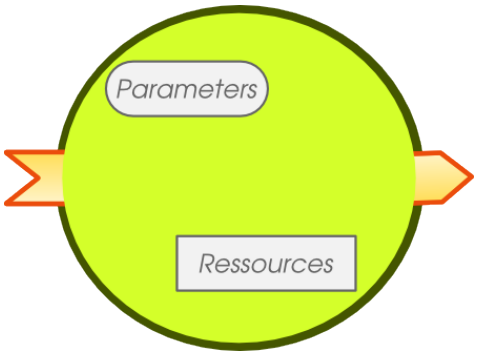
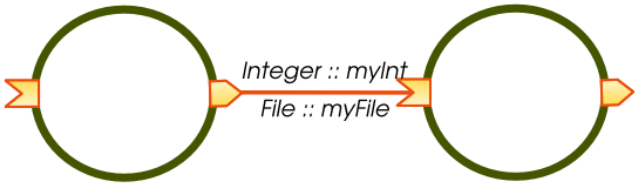
Integrating a Task in workflow requires:

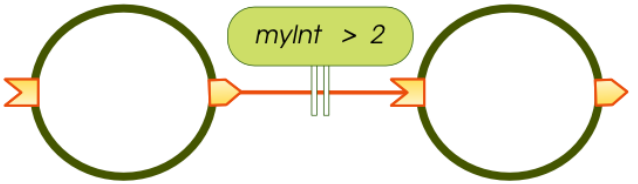
- parameterizing it (providing a Groovy script, a Netlogo script, a command line for launching a model...)
- optionally associating resources with it (libraries, data files, executable files...)



Transitions

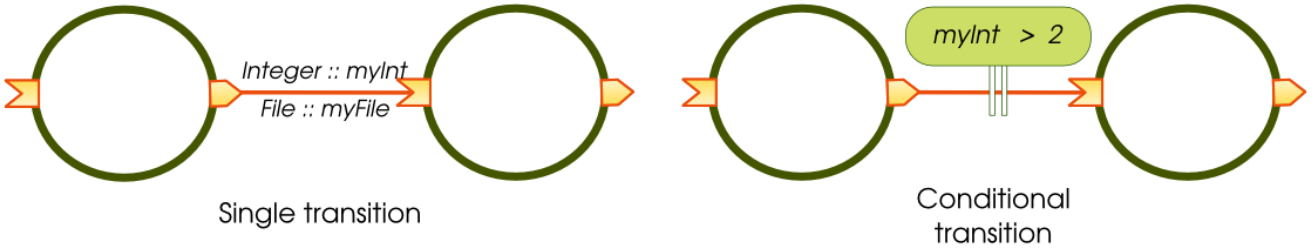


Single transition

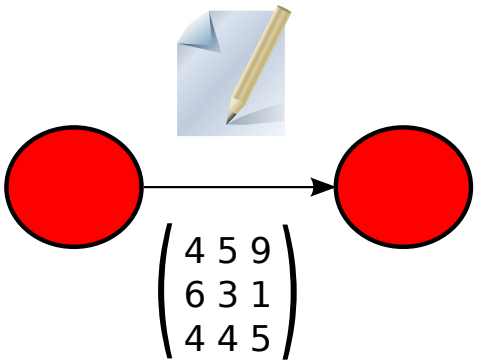


Conditional transition

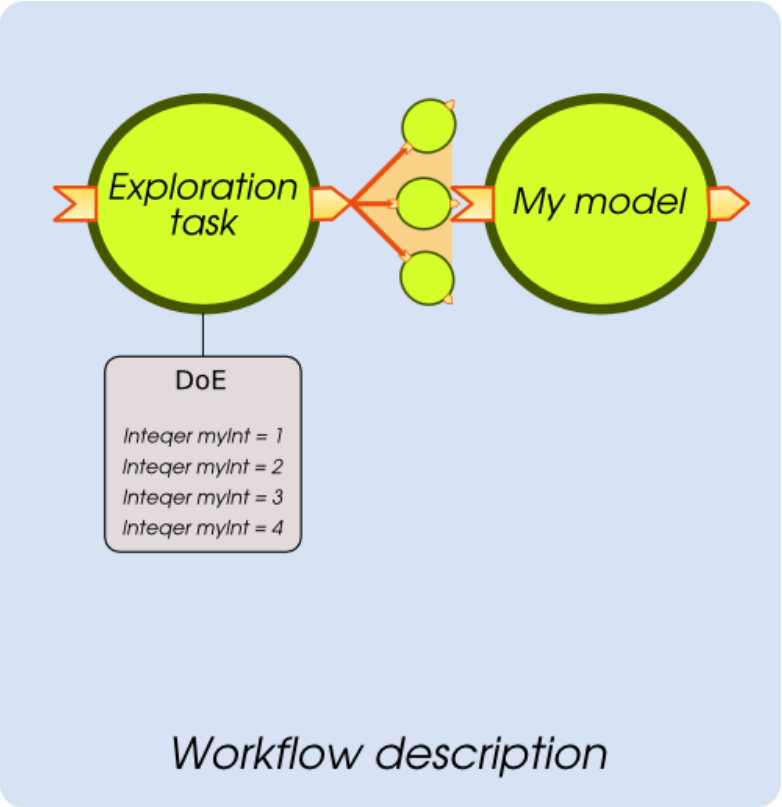
Transitions



OpenMOLE **manages data and file transfers** between the workflow tasks (executed locally, or remotely on an execution node of a cluster or a grid)



Exploration transition



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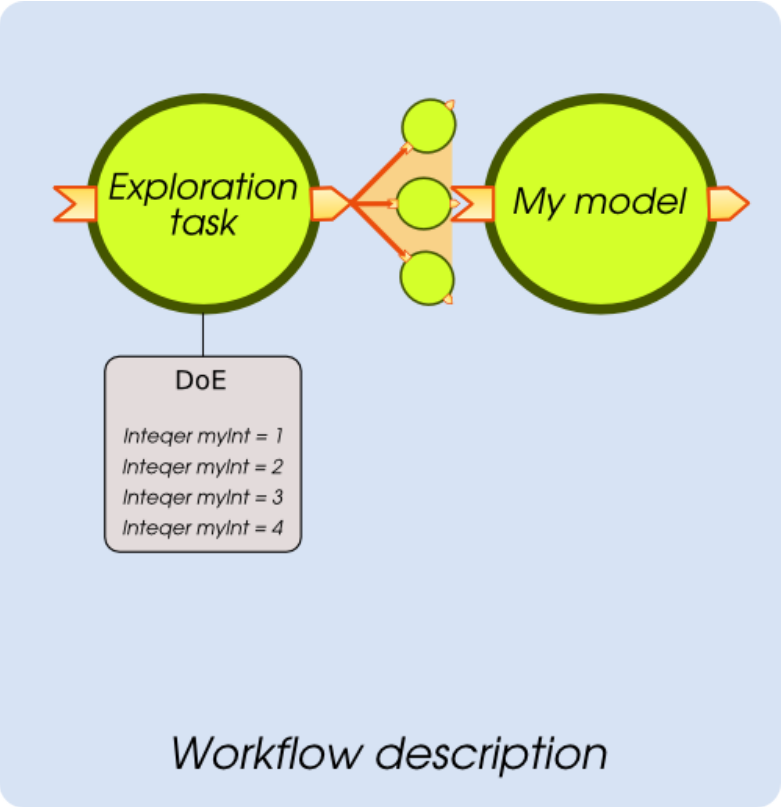
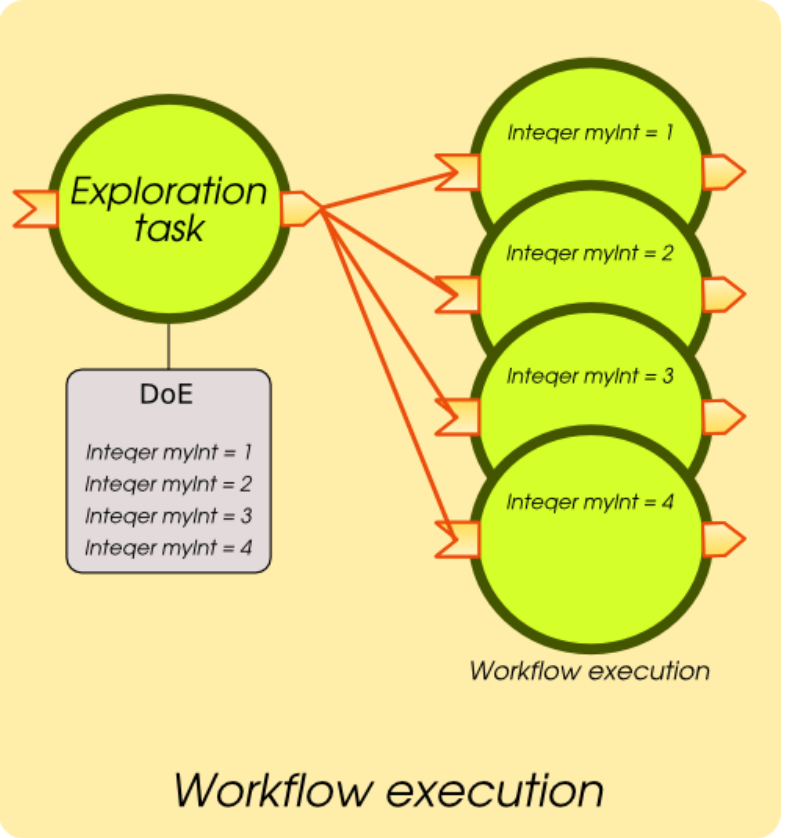
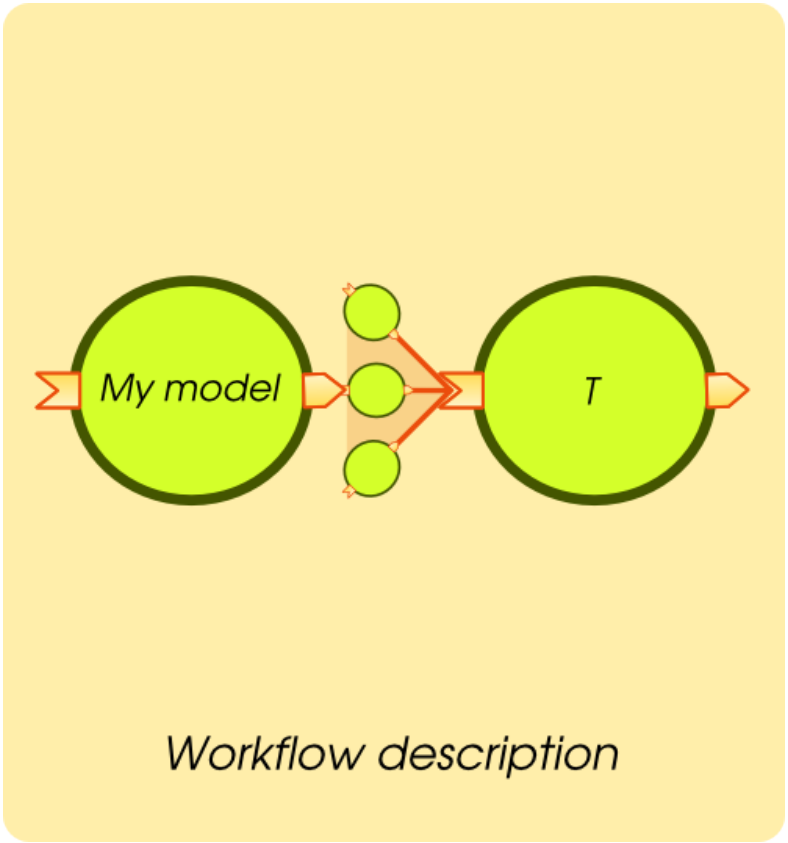




Aggregation transition



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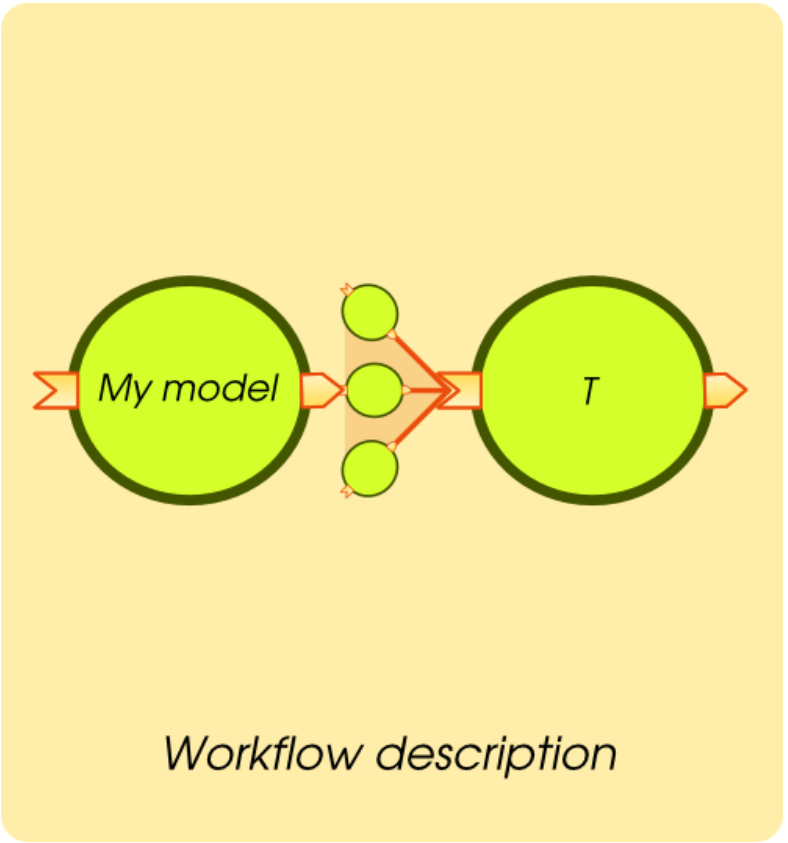

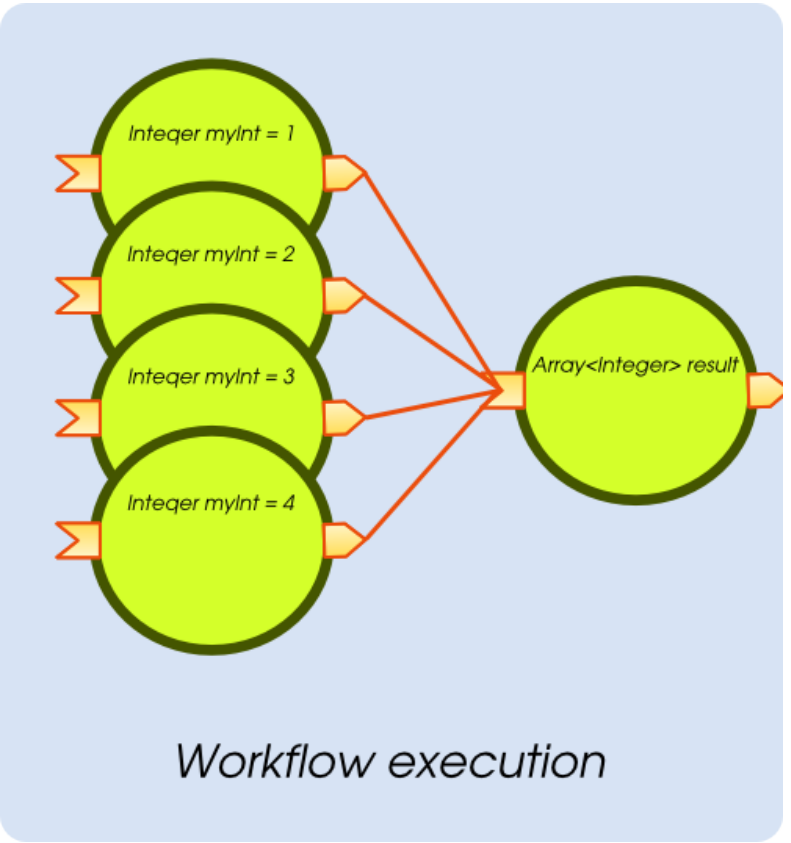

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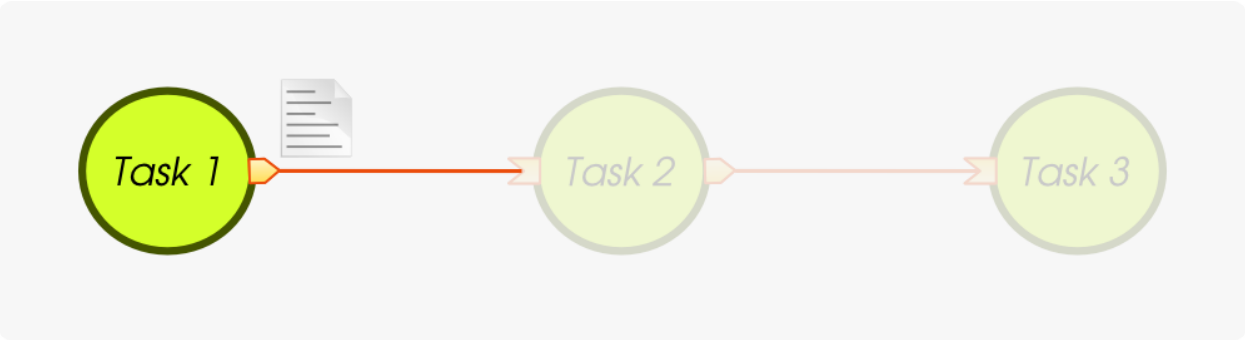
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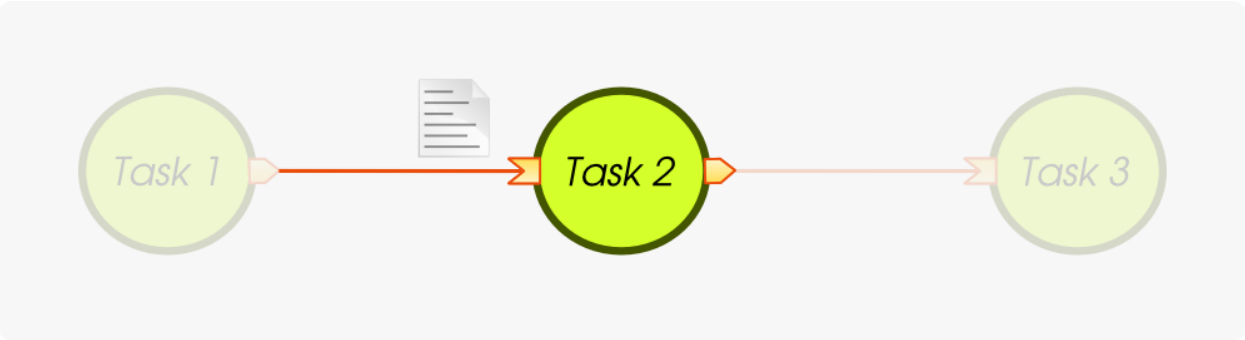
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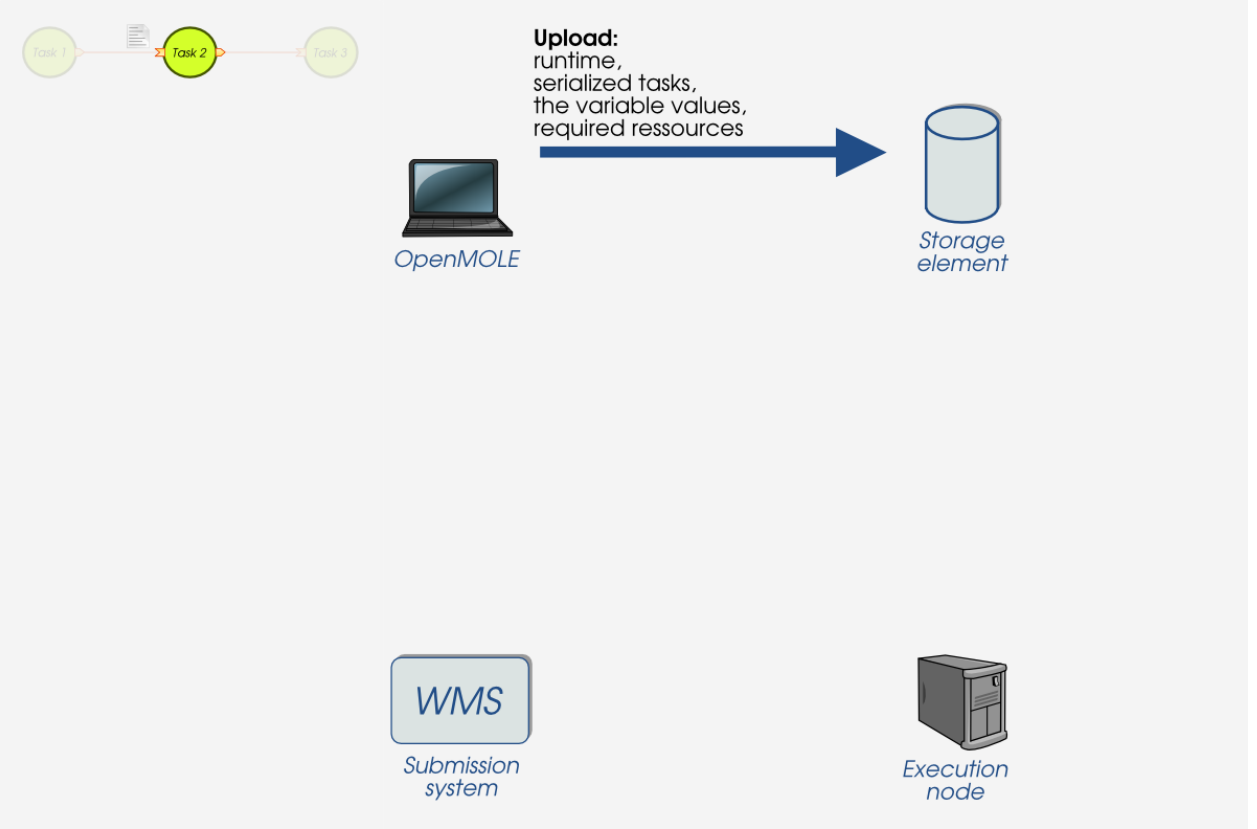
OpenMOLE

Storage element

WMS

Submission system

Execution node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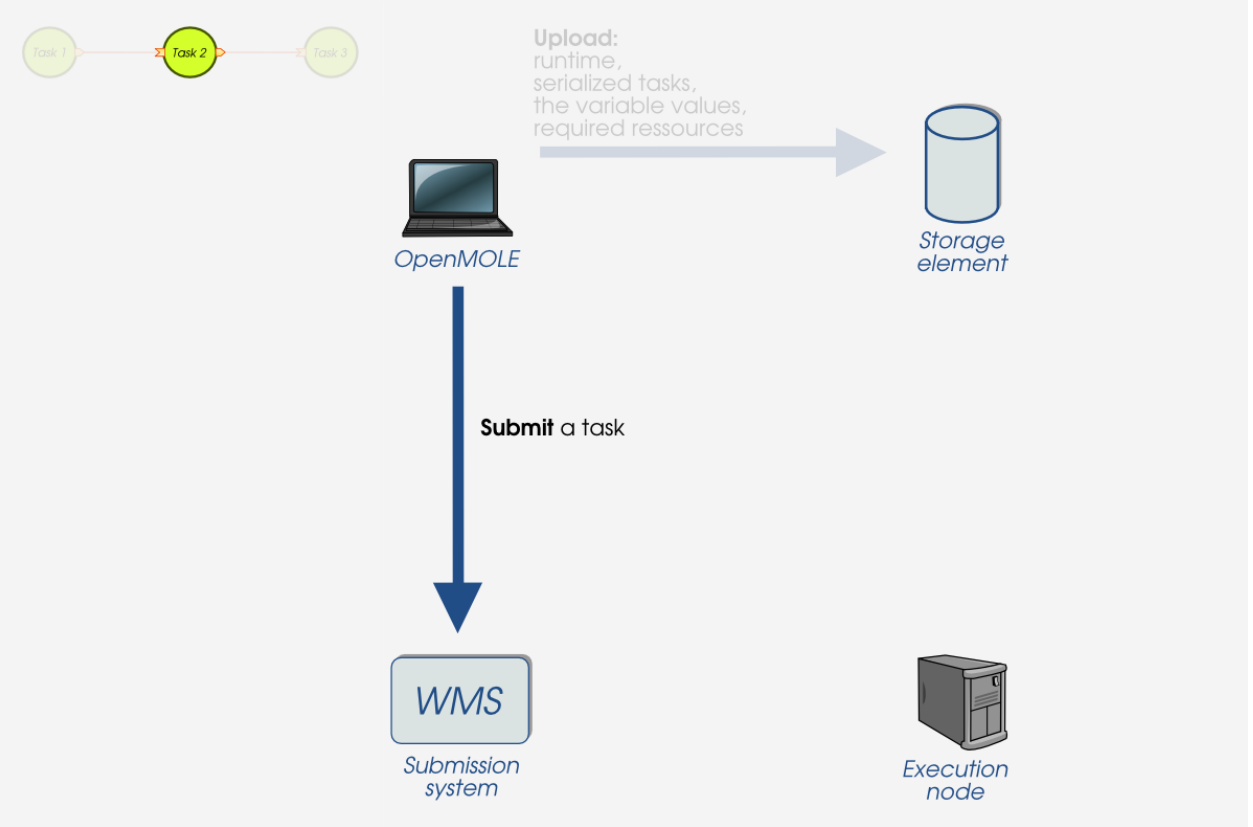
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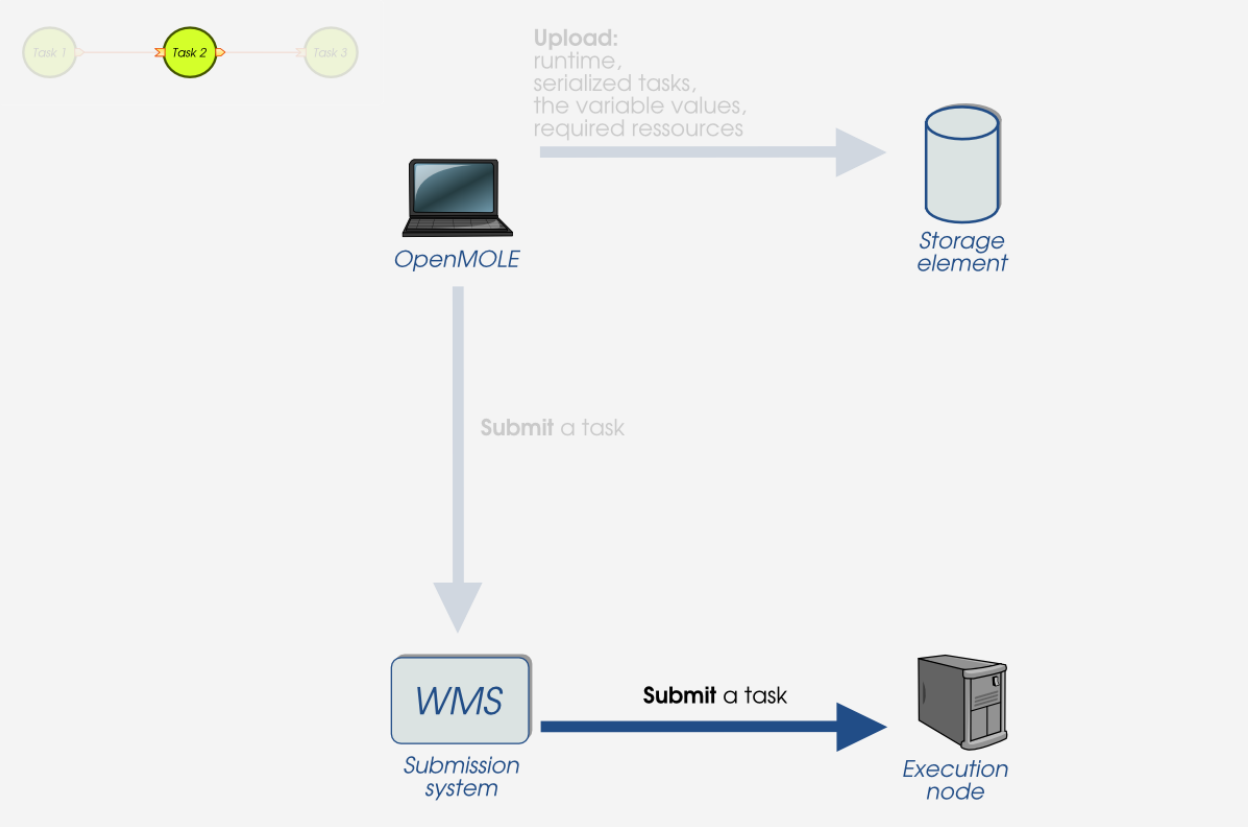
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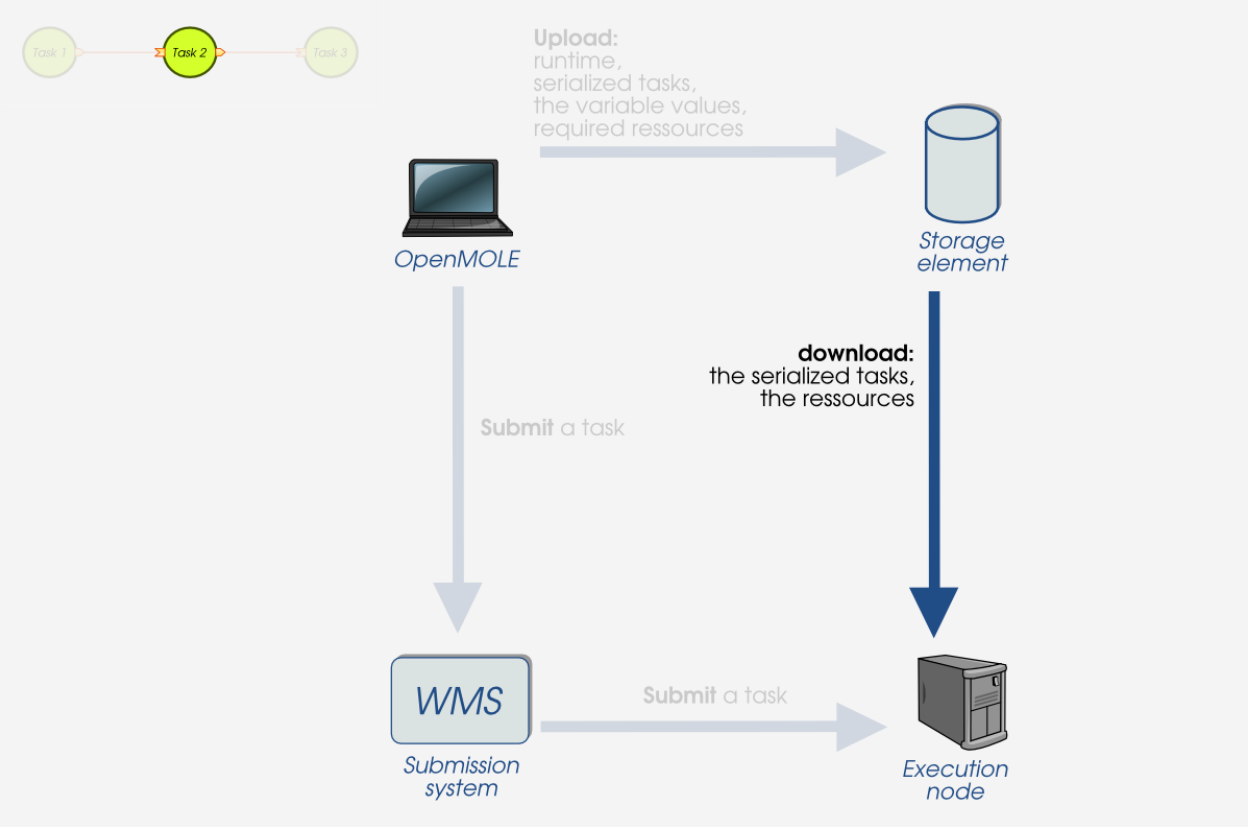
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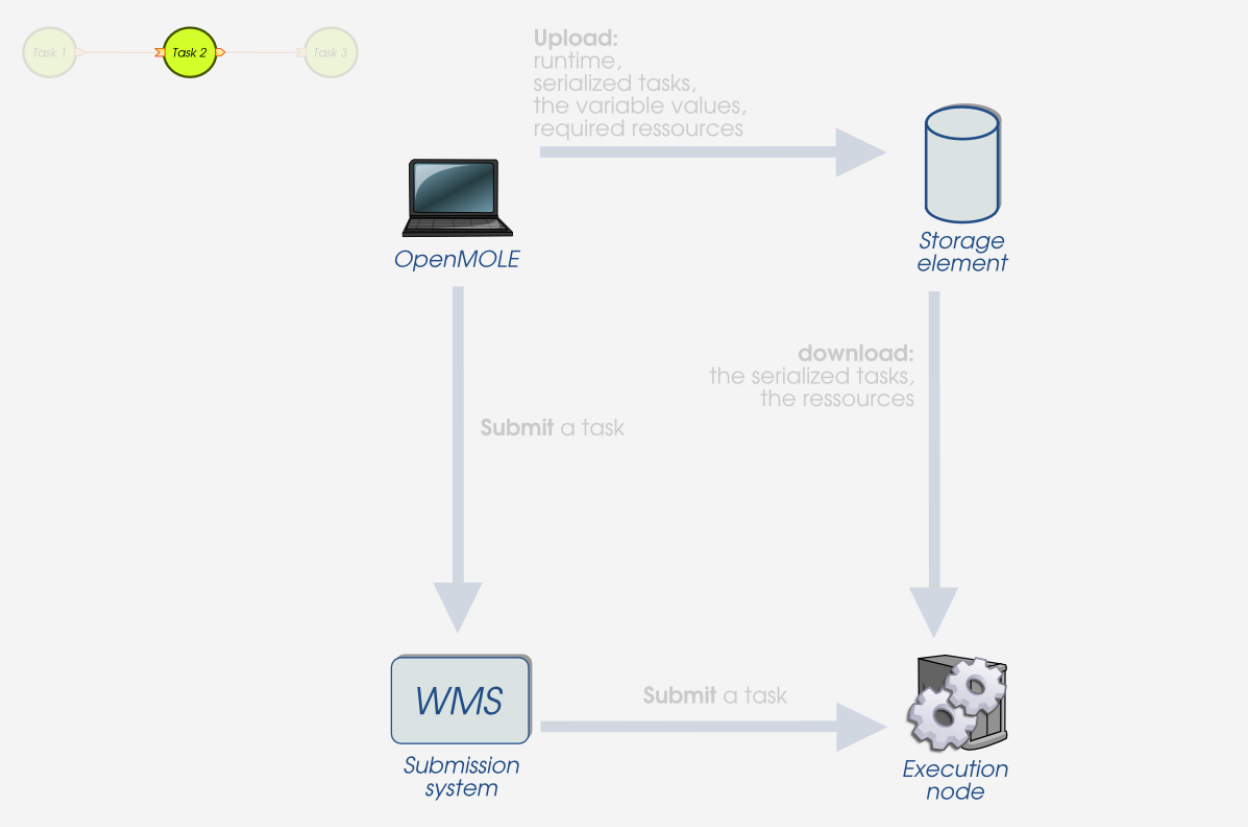
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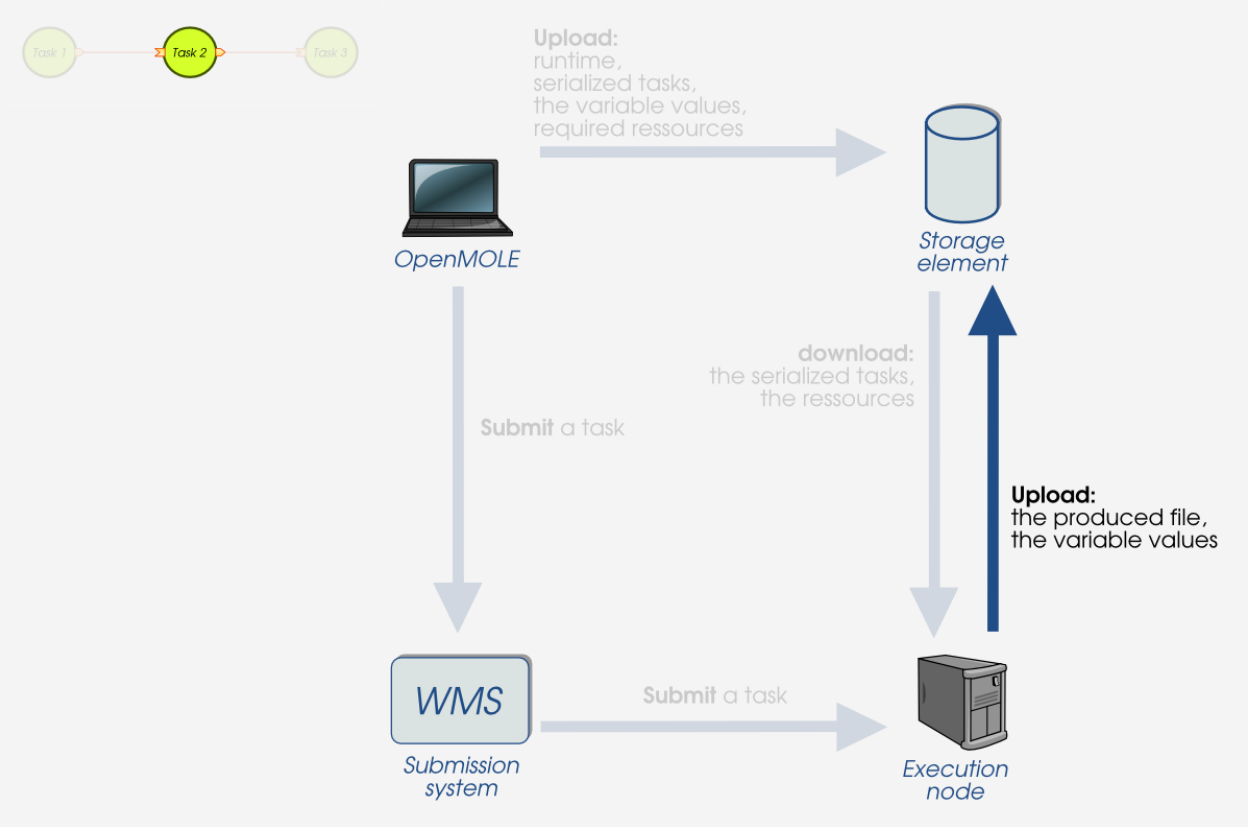
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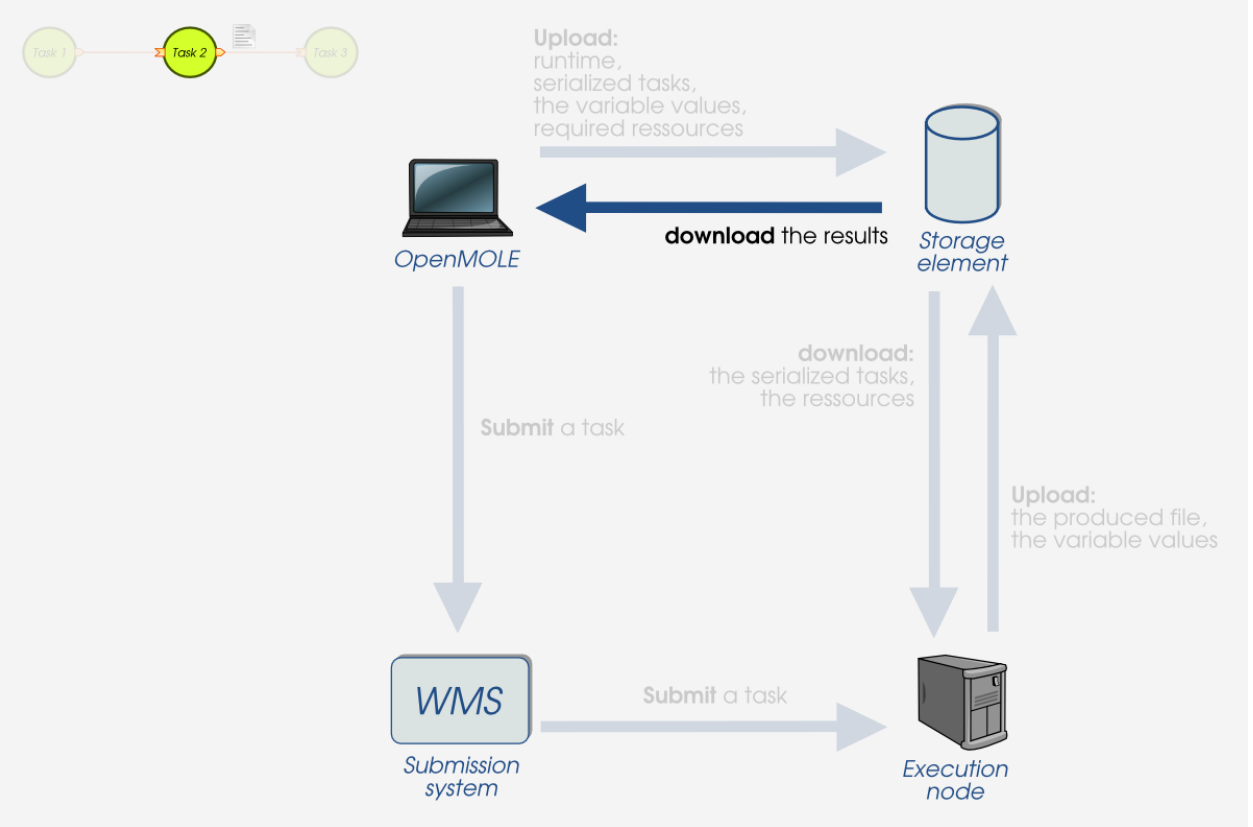
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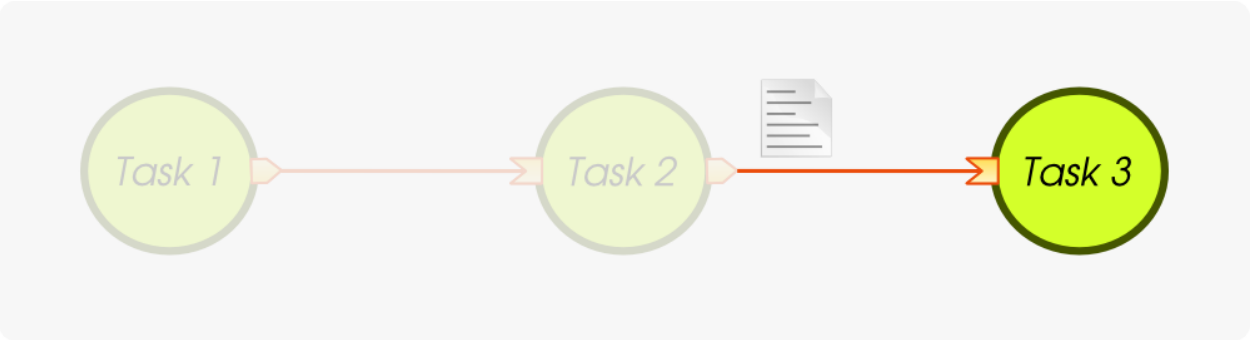
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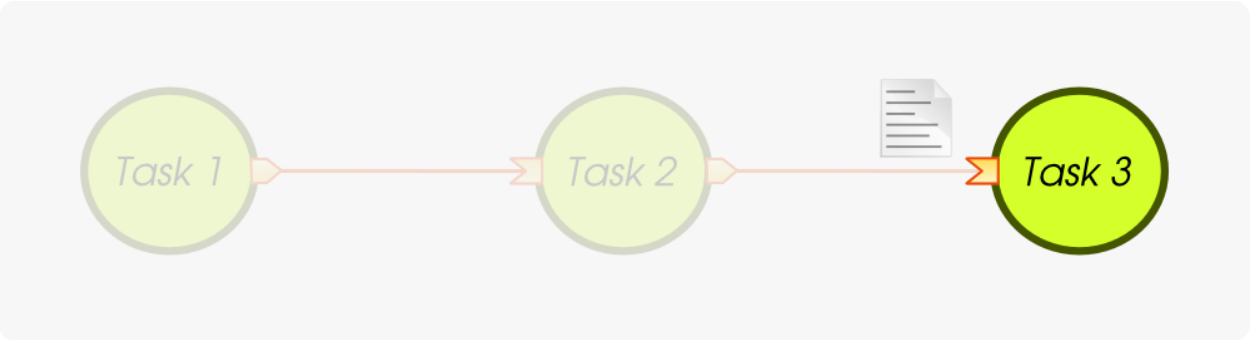
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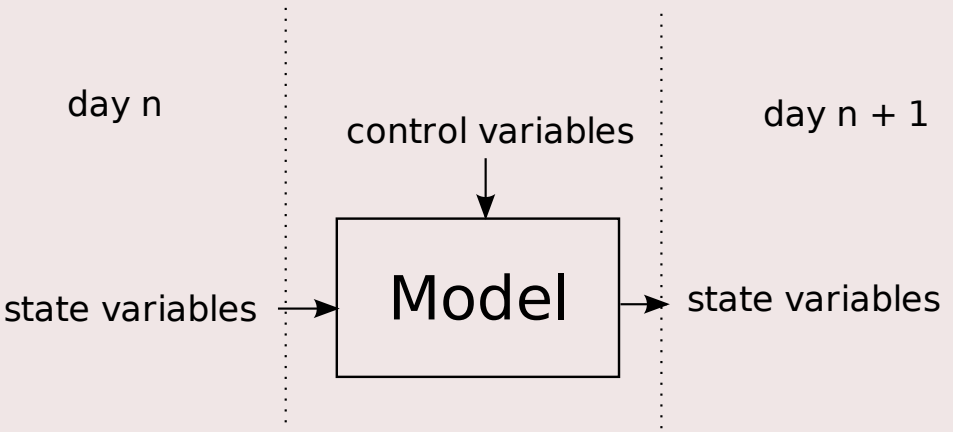
The viability algorithm

The model

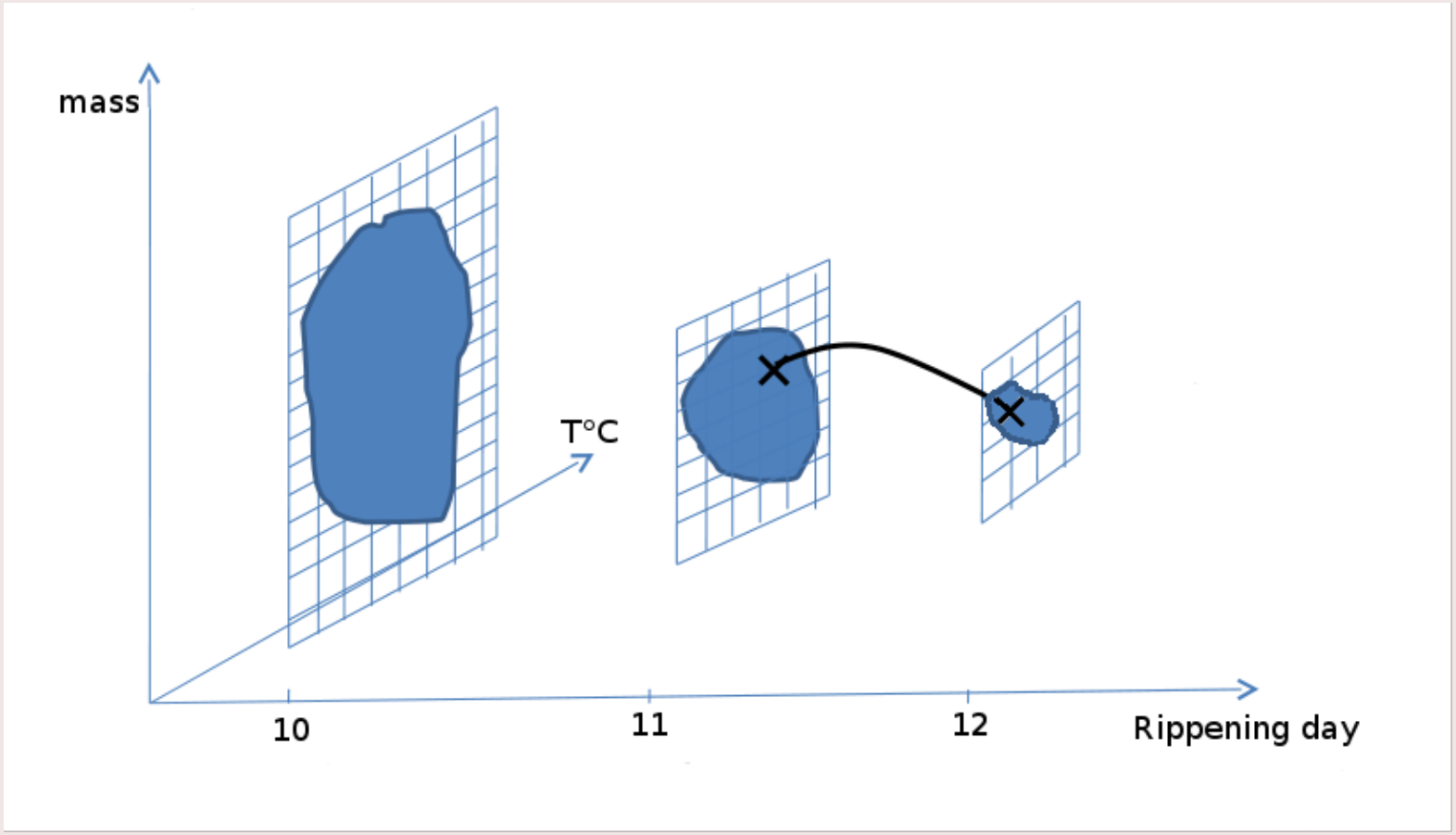
Controllable model of Camembert cheese ripening:

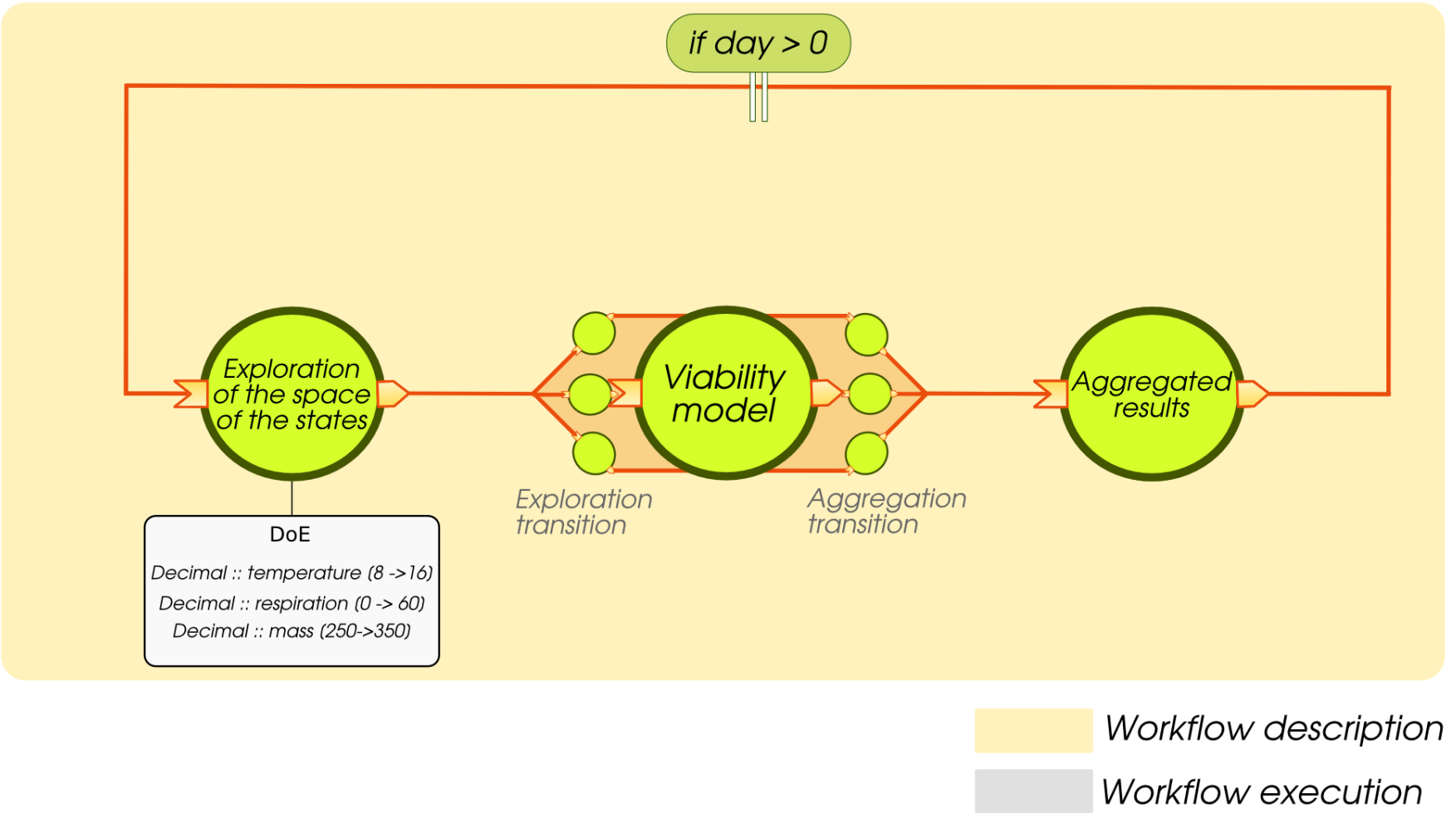


State = mass, micro-organisms activity and surface temperature
Control = temperature and humidity in the ripening chamber.

The viability algorithm

The tube computation

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Viability model
Aggregated results
Exploration transition
Aggregation transition
DoE
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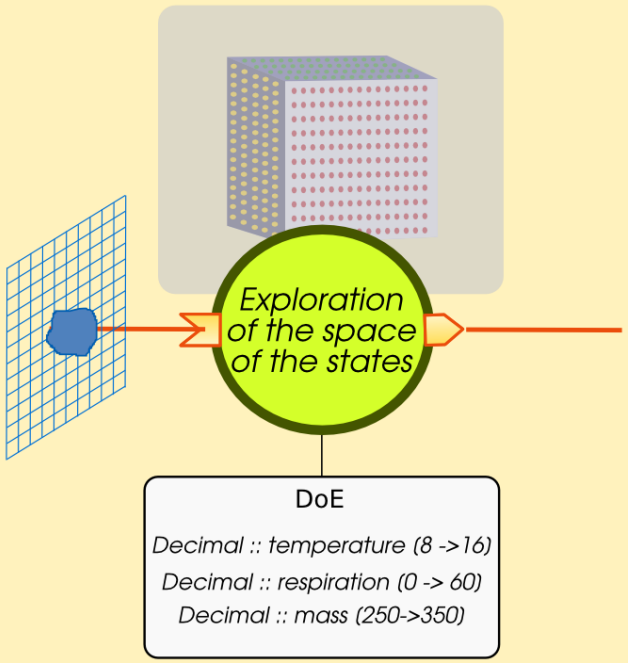
Decimal :: respiration (0 -> 60)
Decimal :: mass (250->350)
Workflow description
Workflow execution



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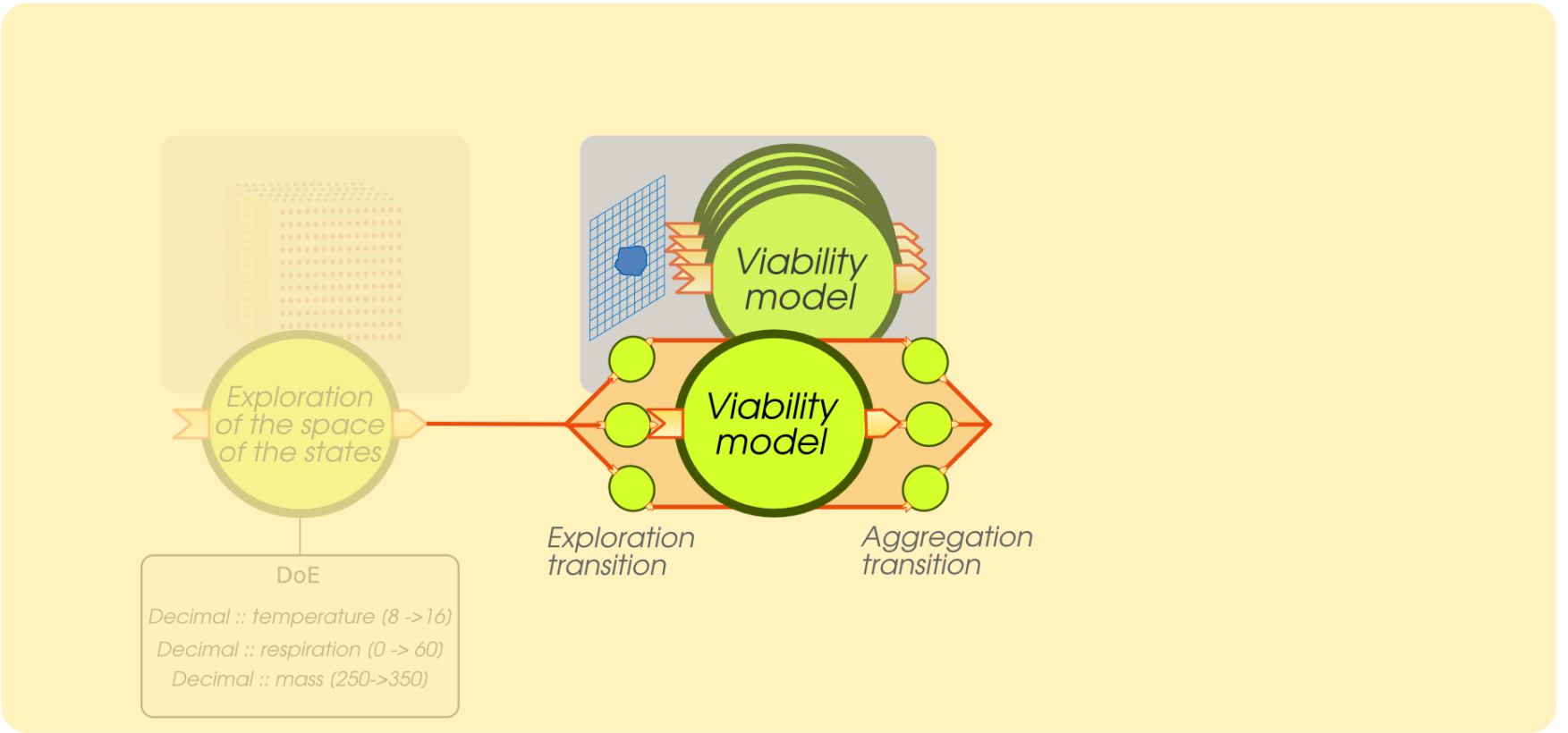

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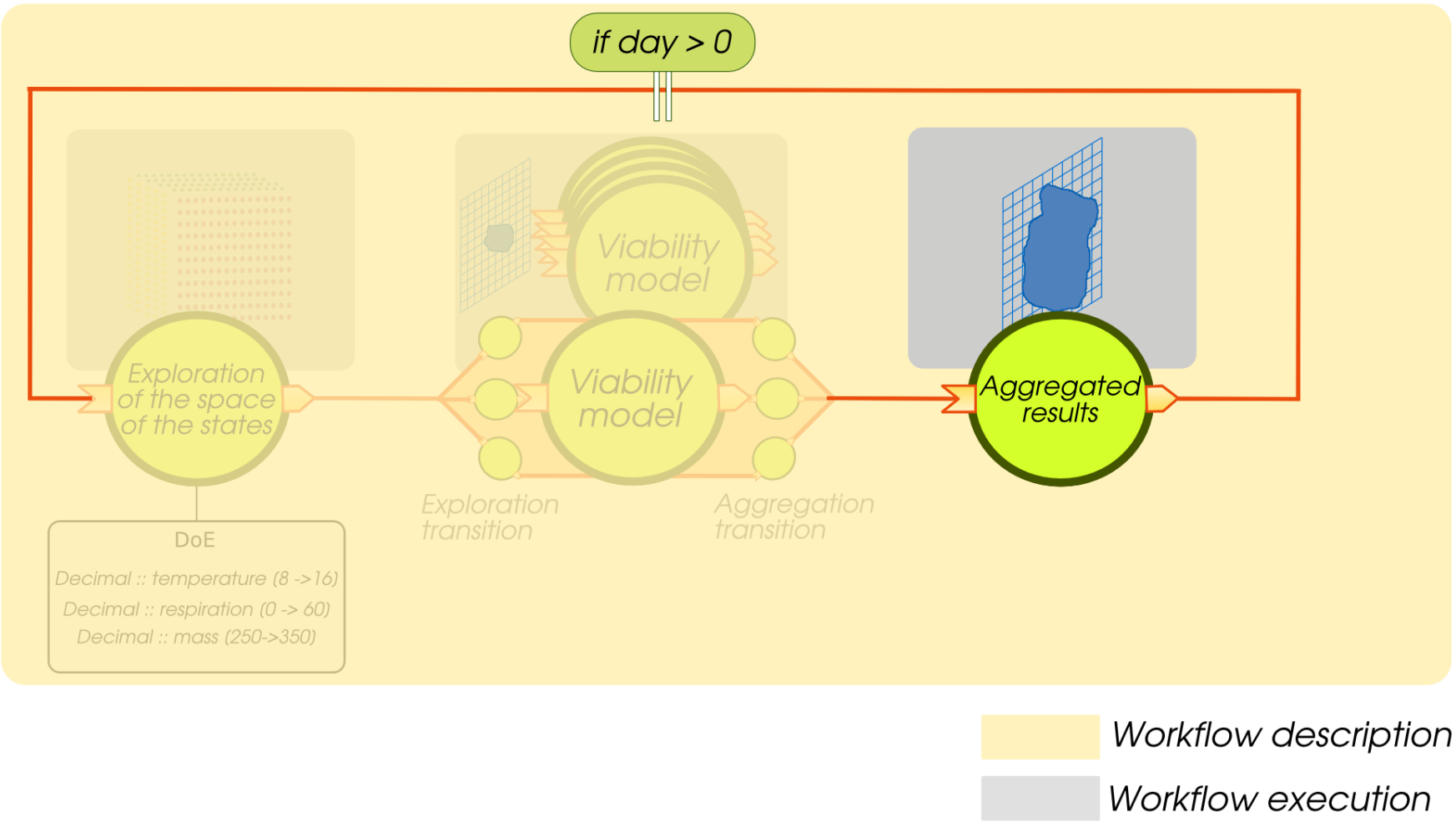
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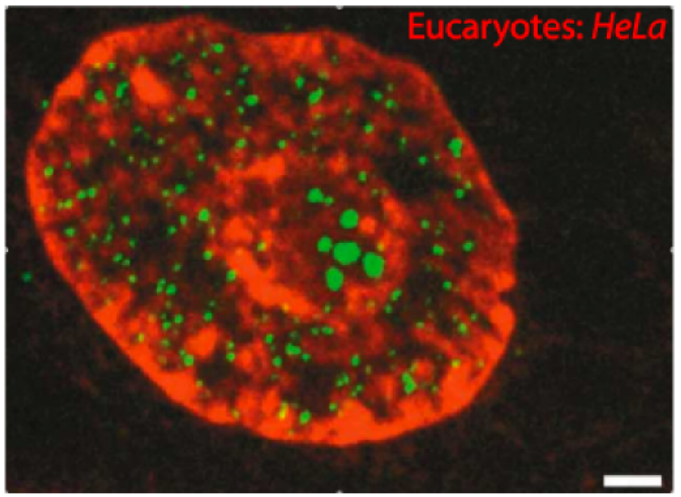
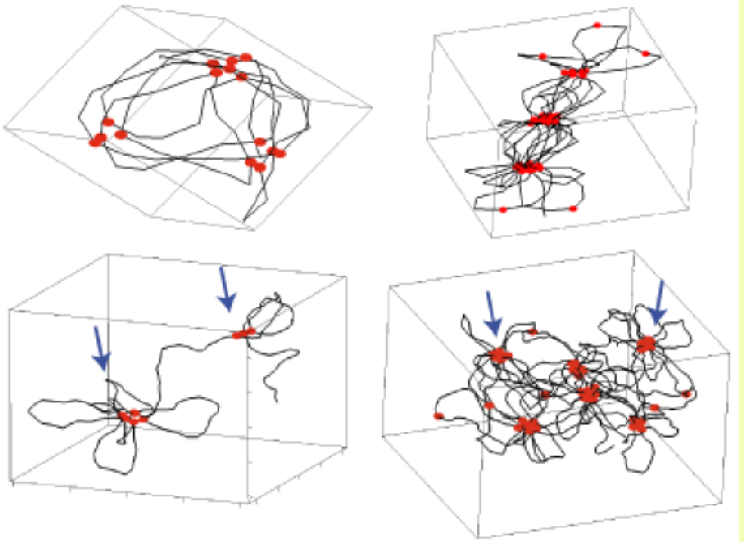
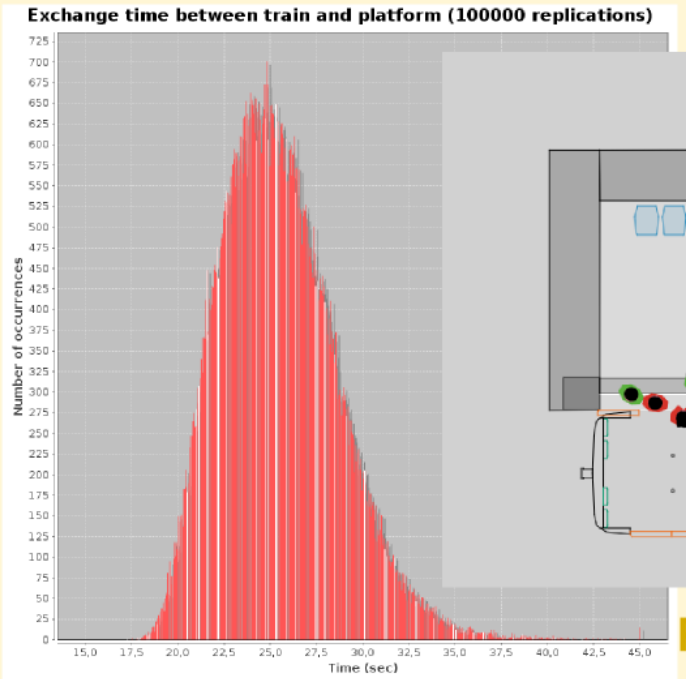
Bioinformatics

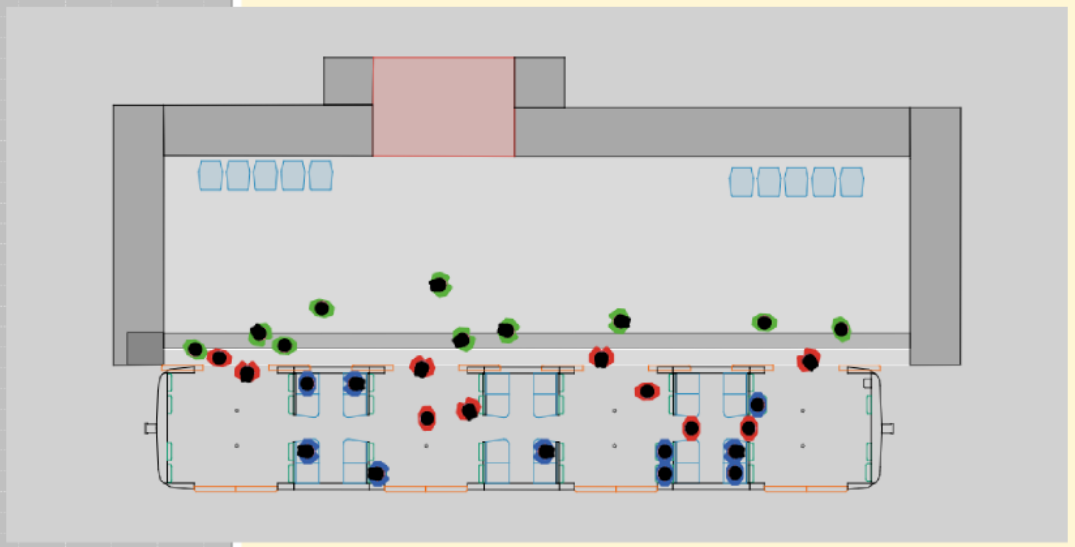




Chromosome structuring

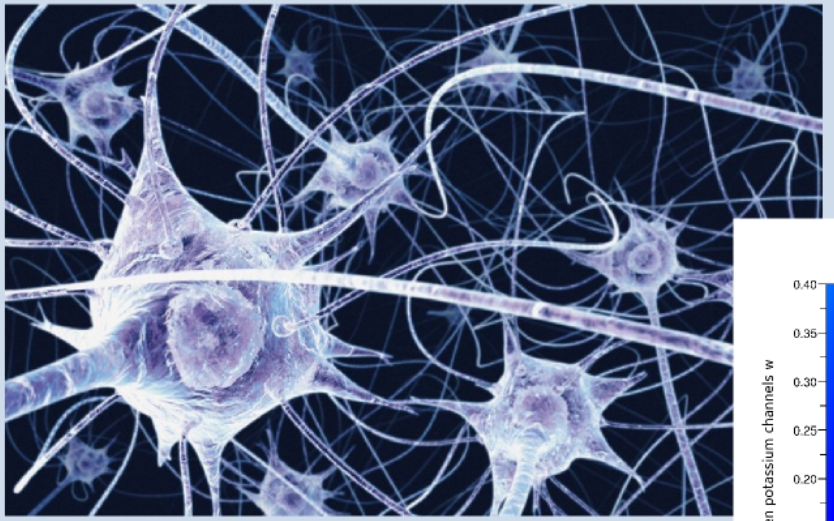
Agent based model



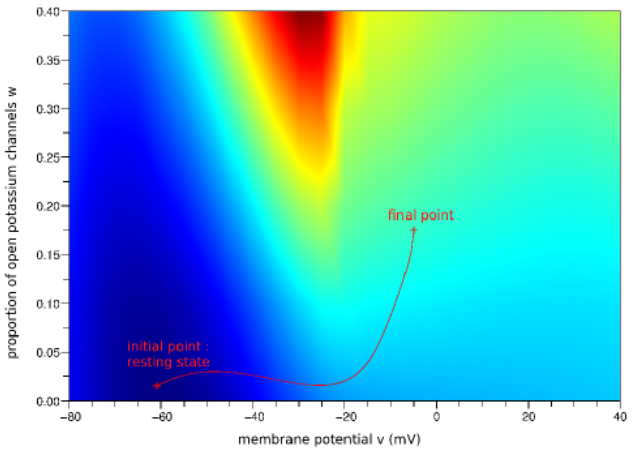


Passenger exchanges between trains and platforms

Neurosciences



Neuronal computing



Projects:

Computer science	multi-scale percolation in collaboration	**IRD institute**
Modeling theory	predator-prey model of savanna	**PATRES European project and CEMAGREF**
Food engineering	the viability theory to control complex food process	**INCALIN French research project and INRA**
Physics	self-propelled particles	**Complex System Institute**

Coming soon:

Image processing	cell tracking on embryos	**Bioemergences European research project**
Optimization	multi-objective optimization using distributed evolutionary algorithms	**DREAM European research project**
Image processing	functional analysis of brain images	**Curie institute**

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Acknowledgement & Question

We would like to thanks the JSAGA project and in particular Sylvain Reynaud (IN2P3) for his help.

Hello world!

```
helloFile = new Prototype<File>("helloFile", File.class)
generateTask = new GroovyTask("Generate file")
generateTask.setCode("helloFile = workspace.newTmpFile();\nhelloFile.write('Hello from groovy');\n")
generateTask.addOutput(helloFile)

displayTask = new GroovyTask("Display file")
displayTask.setCode("println helloFile.text")
displayTask.addInput(helloFile)

generateCapsule = new TaskCapsule(generateTask)
new SingleTransition(generateCapsule, new TaskCapsule(displayTask))
new Mole(generateCapsule).run()
```