

OpenMOLE: a grid enabled workflow platform

Romain REUILLON, Mathieu LECLAIRE

romain.reuillon@openmole.org

mathieu.leclaire@openmole.org

www.openmole.org



June 2, 2010

Introduction

Even though computational grids is a solution to compute problems unsolvable otherwise, grid usage is widely established a tricky domain.

Introduction

Even though computational grids is a solution to compute problems unsolvable otherwise, grid usage is widely established a tricky domain.

Hopefully, categories of problems exhibit naturally **parallel aspects**:

- design of experiments,
- evolutionary algorithms,
- stochastic simulations with many replications,
- ...

Introduction

Even though computational grids is a solution to compute problems unsolvable otherwise, grid usage is widely established a tricky domain.

Hopefully, categories of problems exhibit naturally **parallel aspects**:

- design of experiments,
- evolutionary algorithms,
- stochastic simulations with many replications,
- ...

⇒ It is possible to develop a **generic software framework** for distributing naturally parallel application.

Outline

- 1 Genesis
- 2 OpenMOLE
- 3 Task delegation
- 4 Scientific projects

From a sequential approach...

OpenMOLE was originally a platform for experimenting on models on a single computer (SimExplorer).

From a sequential approach...

OpenMOLE was originally a platform for experimenting on models on a single computer (SimExplorer).

Central concepts;

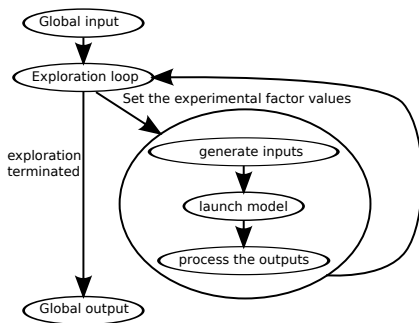
- tasks (software components),
- sequence of tasks,
- loops on a sequence of tasks.

From a sequential approach...

OpenMOLE was originally a platform for experimenting on models on a single computer (SimExplorer).

Central concepts;

- tasks (software components),
- sequence of tasks,
- loops on a sequence of tasks.

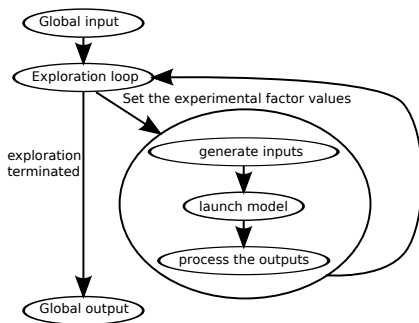


From a sequential approach...

OpenMOLE was originally a platform for experimenting on models on a single computer (SimExplorer).

Central concepts;

- tasks (software components),
- sequence of tasks,
- loops on a sequence of tasks.



These concepts were inherently **sequential** !

... to a distributed approach.

The project was redesigned from scratch in October 2008.

... to a distributed approach.

The project was redesigned from scratch in October 2008.

A workflow approach was chosen because it provides both:

- sequential relationships between tasks where needed,

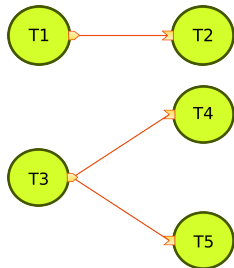


... to a distributed approach.

The project was redesigned from scratch in October 2008.

A workflow approach was chosen because it provides both:

- sequential relationships between tasks where needed,
- naturally parallel representations of algorithms.

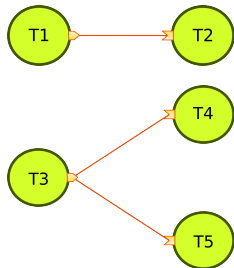


... to a distributed approach.

The project was redesigned from scratch in October 2008.

A workflow approach was chosen because it provides both:

- sequential relationships between tasks where needed,
- naturally parallel representations of algorithms.



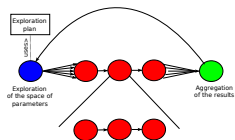
Untie distributed algorithms and execution environments = environment agnostic distributed algorithms.

Outline

- 1 Genesis
- 2 OpenMOLE**
- 3 Task delegation
- 4 Scientific projects

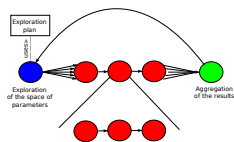
OpenMOLE:

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



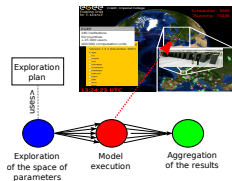
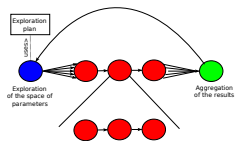
OpenMOLE:

- allows **the definition of complex workflows** for model exploration,
- **manages the execution** of these workflows on the user desktop PC,



OpenMOLE:

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

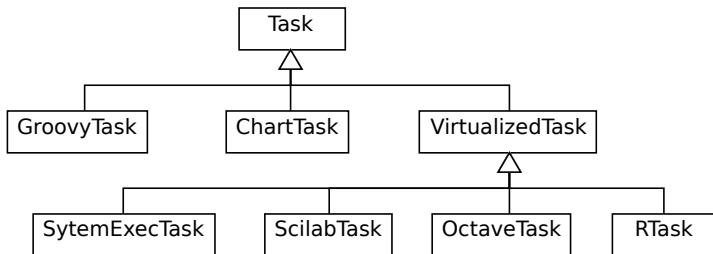
Definition

A task describes a portable computation which can be executed on any execution environment. Task is polymorphic and extensible.

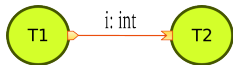
Tasks

Definition

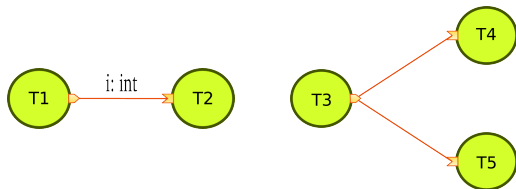
A task describes a portable computation which can be executed on any execution environment. Task is polymorphic and extensible.



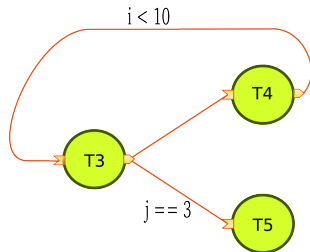
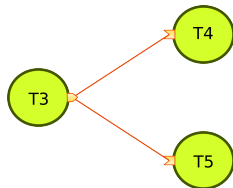
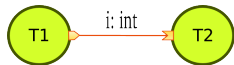
Simple Transitions



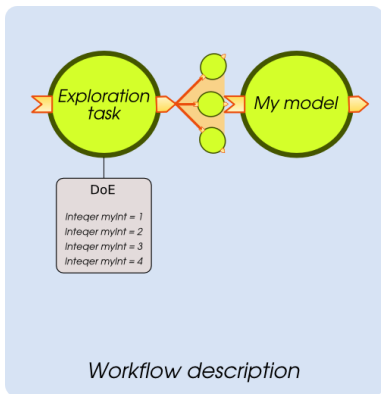
Simple Transitions



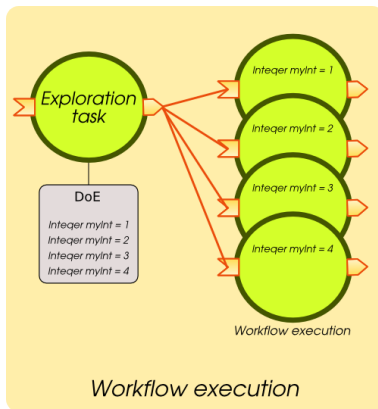
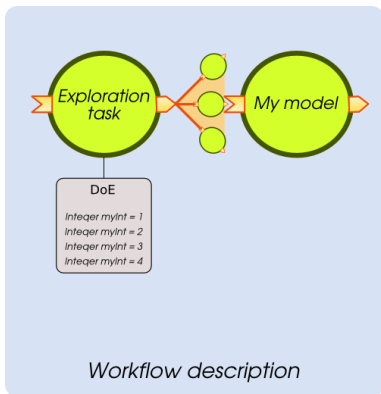
Simple Transitions



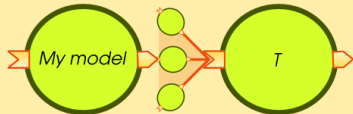
Exploration transition



Exploration transition

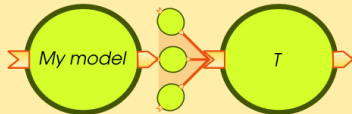


Aggregation transition

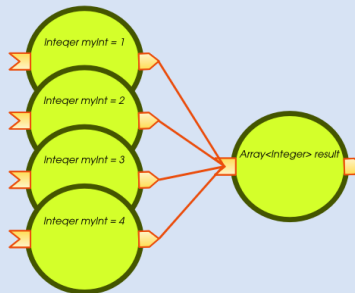


Workflow description

Aggregation transition



Workflow description



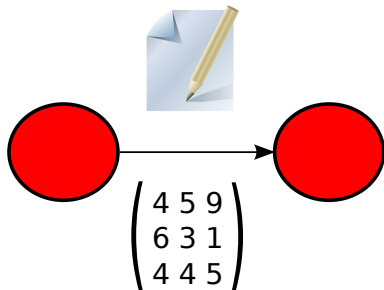
Workflow execution

Outline

- 1 Genesis
- 2 OpenMOLE
- 3 Task delegation**
- 4 Scientific projects

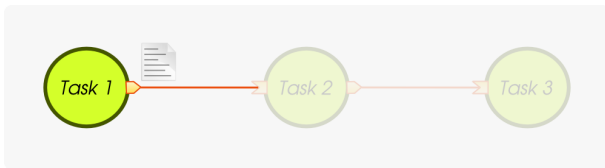
OpenMOLE allows declarative delegation of tasks on distributed execution environments.

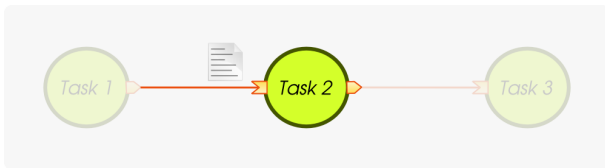
OpenMOLE **manages data and file transfers** between the workflow tasks (executed locally, or remotely on an execution node of a cluster or a grid)



Delegation of a task on EGEE









OpenMOLE



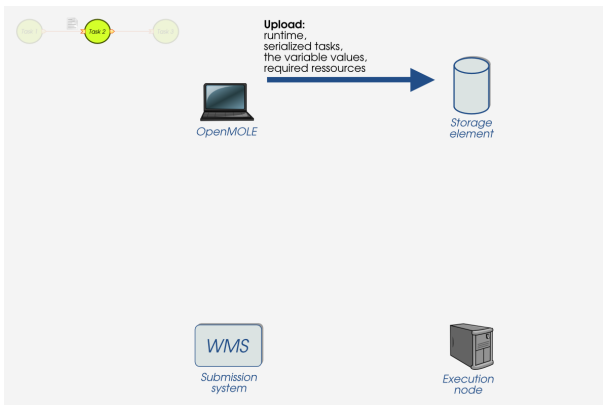
Storage
element

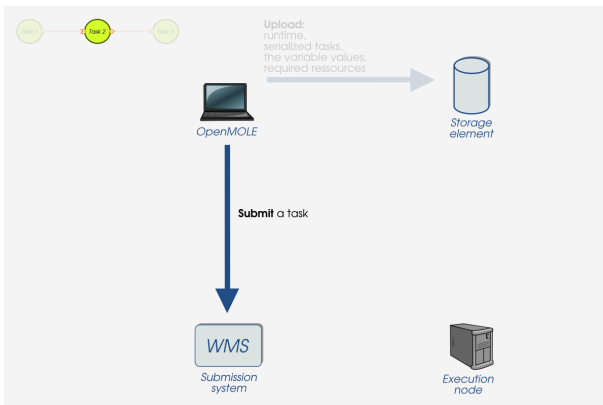


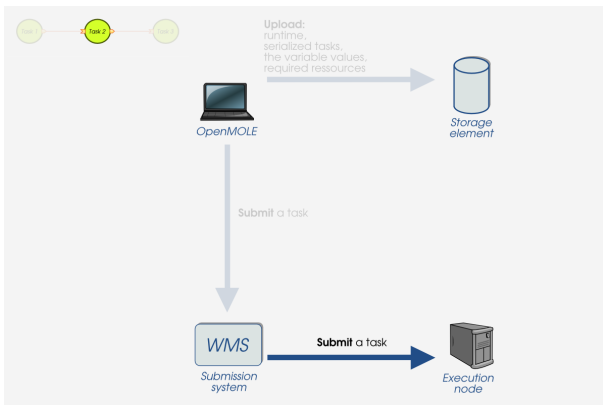
Submission
system

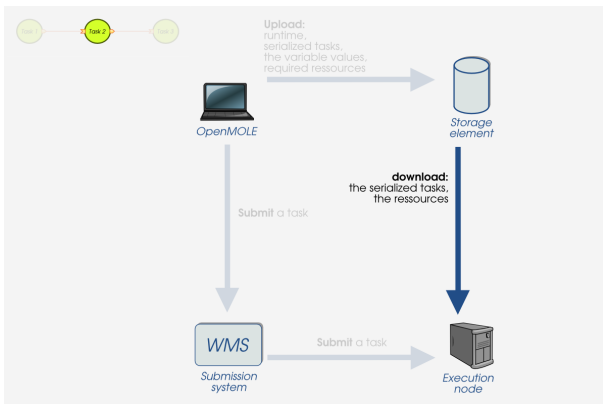


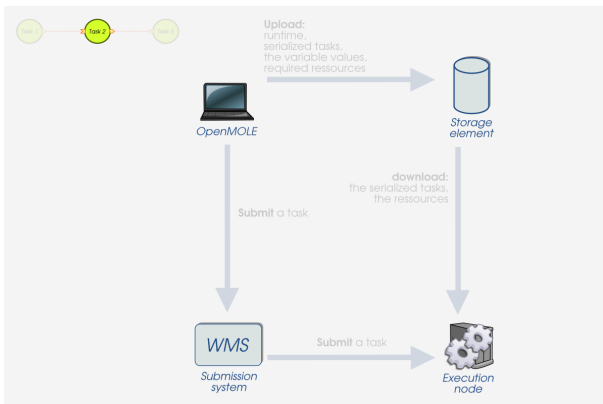
Execution
node

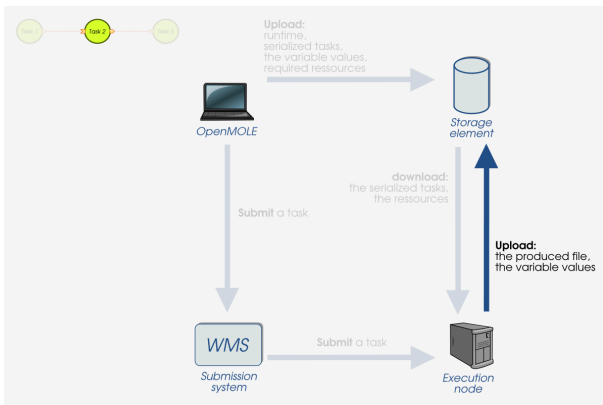


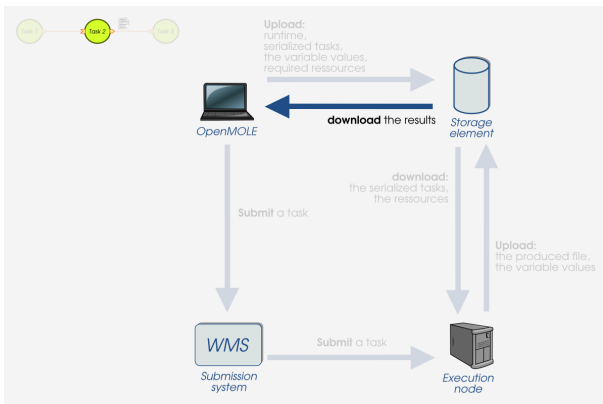


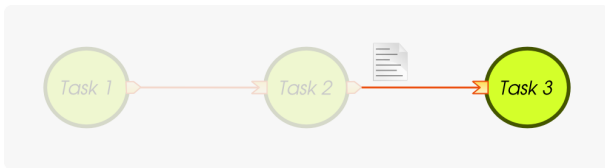


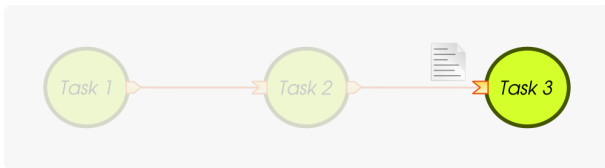










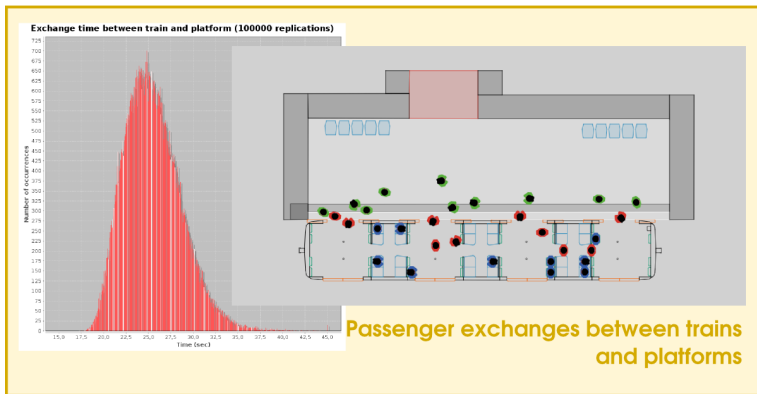


Outline

- 1 Genesis
- 2 OpenMOLE
- 3 Task delegation
- 4 Scientific projects**

Drawing distribution of random variables

Agent based model



Projects:

Computer science	multi-scale percolation in collaboration	IRD institute
Modeling theory	predator-prey model of savanna	PATRES European project and CEMAGREF
Viability	viability applied to complex food process	INCALIN French research project and INRA
Optimization	multi-objective optimization using distributed evolutionary algorithms	DREAM European research project
Physics	self-propelled particles	Complex System Institute

Coming soon:

Image processing	cell tracking on embryos	Bioemergences European research project
Image processing	functional analysis of brain images	INSERM

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Advanced features:

- Extensible platform through plugins (30 plugins and the number is growing).

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Advanced features:

- Extensible platform through plugins (30 plugins and the number is growing).
- Statistically sounded over-submission algorithms for efficient grid execution.

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Advanced features:

- Extensible platform through plugins (30 plugins and the number is growing).
- Statistically sounded over-submission algorithms for efficient grid execution.
- Workflow jobs grouping in a single grid job.

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Advanced features:

- Extensible platform through plugins (30 plugins and the number is growing).
- Statistically sounded over-submission algorithms for efficient grid execution.
- Workflow jobs grouping in a single grid job.
- Multi-scale workflows (tasks encapsulating workflows).

Conclusion

The genericity of the platform has been assessed on many real use-cases. OpenMOLE reduces dramatically the engineering time to develop grid-enabled complex system in silico experiments.

Advanced features:

- Extensible platform through plugins (30 plugins and the number is growing).
- Statistically sounded over-submission algorithms for efficient grid execution.
- Workflow jobs grouping in a single grid job.
- Multi-scale workflows (tasks encapsulating workflows).
- Virtualization for portability of legacy software.

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).
- Designing a graphical user interface.

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).
- Designing a graphical user interface.
- Writing consistent user documentation.

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).
- Designing a graphical user interface.
- Writing consistent user documentation.

Perspectives:

- Generic workflow patterns for scientific algorithms.

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).
- Designing a graphical user interface.
- Writing consistent user documentation.

Perspectives:

- Generic workflow patterns for scientific algorithms.
- Collaborative development on workflows (decentralized versioning system).

Conclusion

Where we are now:

- Packaging a command line user interface version (almost done).
- Designing a graphical user interface.
- Writing consistent user documentation.

Perspectives:

- Generic workflow patterns for scientific algorithms.
- Collaborative development on workflows (decentralized versioning system).
- Meta-data management.

Acknowledgement & Question

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



```

textVariable = new Prototype("text", String)

assignTask = new GroovyTask("Assign_task")
assignTask.setCode(" text == 'Hello_world!' ")
assignTask.addOutput(textVariable)

helloTask = new GroovyTask("Sample_groovy_task")
helloTask.setCode(" println text ")
helloTask.addInput(textVariable)

assignTaskCapsule = new TaskCapsule(assignTask)
helloTaskCapsule = new TaskCapsule(helloTask)
ex = new Mole(assignTaskCapsule, helloTaskCapsule).createExecution()
ex.start()

```

