Cloud-based Scientific Workflow Management

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1. Data is generated and collected

2. Data is first analyzed by programs MAFFT, Muscle...

3. Large volume of data are produced...

4. ...which need to be processed by a virtual cluster using MG and RAxML

5. Final results are analyzed

Some initiatives propose solutions for managing parallel executions workflows in cloud environments

HPC Scientific Cloud Scenario

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Challenges

Hello,

I have noticed that one or more of your instances is running on a host that is degraded due to hardware failure. The host needs to undergo maintenance and will be taken down after 12:00 GMT on 2011-12-26. If you do not take action before this time, they will be terminated at this point.

The risk of your instances failing is increased at this point. We cannot determine the health of any applications running on these instances. We recommend that you take appropriate action.

EC2 instances have been scheduled for some patch updates. Most reboots complete within minutes, depending on your instance configuration. The instance(s) that will be rebooted and your scheduled reboot time(s) are listed below.

<table>
<thead>
<tr>
<th>Region</th>
<th>Instance ID</th>
<th>Maintenance Window</th>
</tr>
</thead>
<tbody>
<tr>
<td>us-east-1</td>
<td>i-03bf4160</td>
<td>2011-12-11 04:00:00 UTC - 2011-12-11 10:00:00 UTC instance-reboot</td>
</tr>
<tr>
<td></td>
<td>i-01bf4162</td>
<td>2011-12-11 04:00:00 UTC - 2011-12-11 10:00:00 UTC instance-reboot</td>
</tr>
</tbody>
</table>

No action is required on your part.
SciCumulus Cloud Engine

• SciCumulus is a parallel workflow engine for cloud environments

• Implements a provenance-based adaptive scheduling heuristic

• Presents a 3-objective weighted cost model considering total execution time, financial cost and reliability
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SciCumulus Architecture

Desktop Layer
- Desktop Setup
  - Workflow
    - Uploader
    - Dispatcher
    - Casturer
    - Downloader

Distribution Layer
- Configuration Repository
- Data Repository
- Global Schema
- Provenance
- Distribution Controller
- Data Summarizer

Execution Layer
- Instance Controller #1
  - Configurator
  - Executor
- Instance Provenance
- Data Repository
- Parameter Sweeper
- Encapsulator
- Scheduler
- Data Fragmenter
- Parameter Sweeper
- Execution Broker
- 1
- 2
- 3.1
- 3.2
- 4
- 5
- 6
- 7
- 8.1
- 8.2
- 9
- 10
- 11
- 12
- 13

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Static Execution

![Graph showing the relationship between the number of virtual cores and execution time for SciCumulus and Hadoop.]
Analysis of the Adaptive Execution

![Graph showing the comparison between Static Scenario and Adaptive Scenario for the number of used virtual cores and the total execution time. The graph indicates that the Adaptive Scenario allows for more dynamic allocation of virtual cores, leading to a more efficient use of resources and reduced total execution time compared to the Static Scenario.](image-url)
Analysis of the Adaptive Execution

Adaptive Execution
Adaptive Execution

Dimensioned Adaptive Execution

![Graph showing the number of used virtual cores over execution time with and without SciDim.]

**Execution time (hours)**

- **Without SciDim**
- **With SciDim**
- **Ideal**

**Number of used virtual cores**

- 0
- 2
- 4
- 6
- 8
- 10
- 12
- 14
- 16
- 18
- 20
Phylogenetic Analysis Workflow

Phylogenomic Analysis Workflow

Data-intensive and CPU-intensive applications

Sequence DB (e.g. Refseq) → MSA Construction → Evolutionary Model Election → Phylogenetic Tree Construction

1. MSA Construction
2. Evolutionary Model Election
3. Phylogenetic Tree Construction

MSA Concatenation

Evolutionary Model

Concatenated MSA

Phylogenomic trees

Individual MSA

Kalign, ClustalW, MAFFT, Muscle, ProbCons

Phylogenetic trees

Sequence DB

(e.g. Refseq)

MSA Construction

Evolutionary Model

Phylogenomic Tree Construction

Phylogenomic trees

Concatenated MSA

BLOSUM62, CPREV, JTT, WAG, RtREV

ModelGenerator

RAXML

Phylogenetic trees

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Phylogenomic Analysis Workflow

SciLightning

• Provides monitoring information for SWfMS
• A non-intrusive approach
• No change in the SWfMS is required
  ▪ Provenance data has to be provided at runtime
• It is based on event notification
• Its components are distributed in the cloud (in several virtual machines) to monitor different scientific workflows on demand.
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SciLightning Architecture

SWfMS -> <Workflow Definition> -> [Coordinator] -> Provenance Repository

Twitter -> <Notification> -> [Analyst] -> <Rules> -> Cartridge

Social 
Mobile 
Google Cloud Messaging for Android

<Notification> -> Monitor -> <Event> -> Rule DB 
<Notification> -> [Analyst] 
<Notification> -> [Analyst] 
<Notification> -> [Analyst] 
<Notification> -> [Analyst] 
<Notification> -> [Analyst]
Dimensioning

• Depending on the cloud provider, there may be several possible VM type combinations to choose and
  ▪ it can be tedious, overpriced and error-prone to be performed manually.

• Use of genetic algorithms to find the best possible amount of VMs for a specific execution

Opportunities

• Model new cloud-based scientific workflows for different experiments (including bioinformaticians in France)

• Extend the proposed approaches for multi-site cloud execution
  ▪ Scheduling
  ▪ Adaptive Execution (auto-scaling)
  ▪ Monitoring
  ▪ Dimensioning
Thank you!