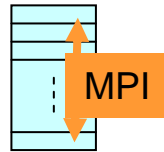

NAREGI JSDL Use Case for Multiple Executables

@GGF17 Tokyo
May, 2006

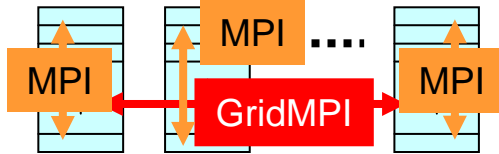
Kazushige Saga
NAREGI-WP1,
National Institute of Informatics

NAREGI Target Job Types

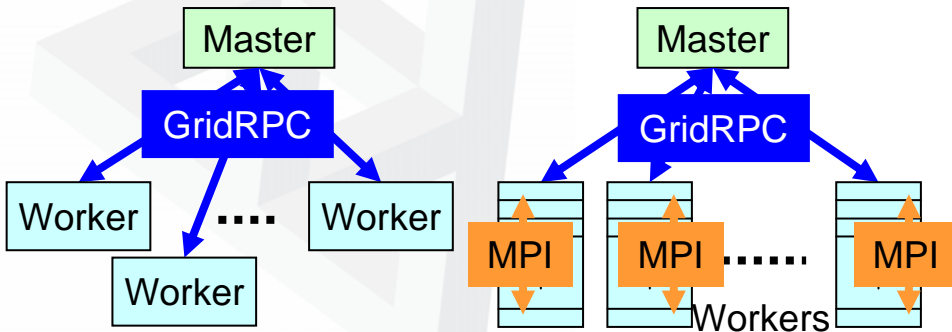
(1) Single MPI executable, running on single system



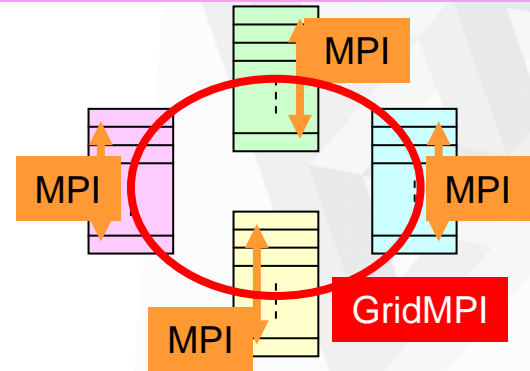
(2) Single MPI executable running across multiple systems on multiple sites



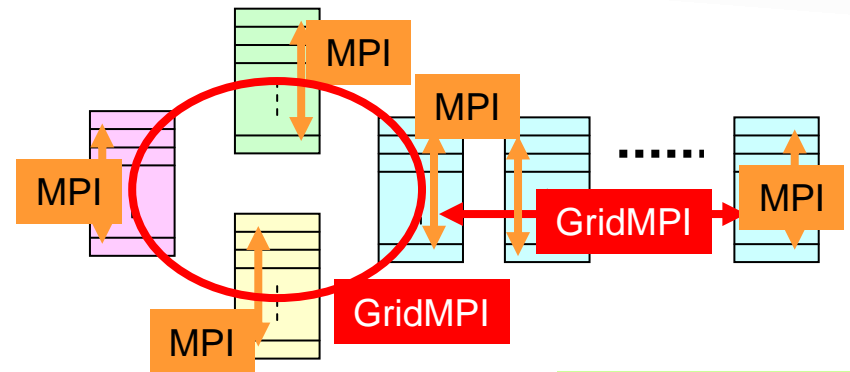
(3) GridRPC worker executables running on multiple systems on multiple sites *



(4) Multiple executables running on multiple systems on multiple sites



(5) Combination of above job types

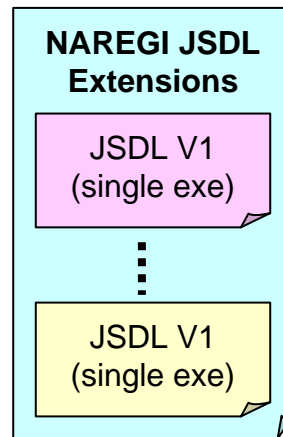


and more...

*: Only workers can be described in current NAREGI specification

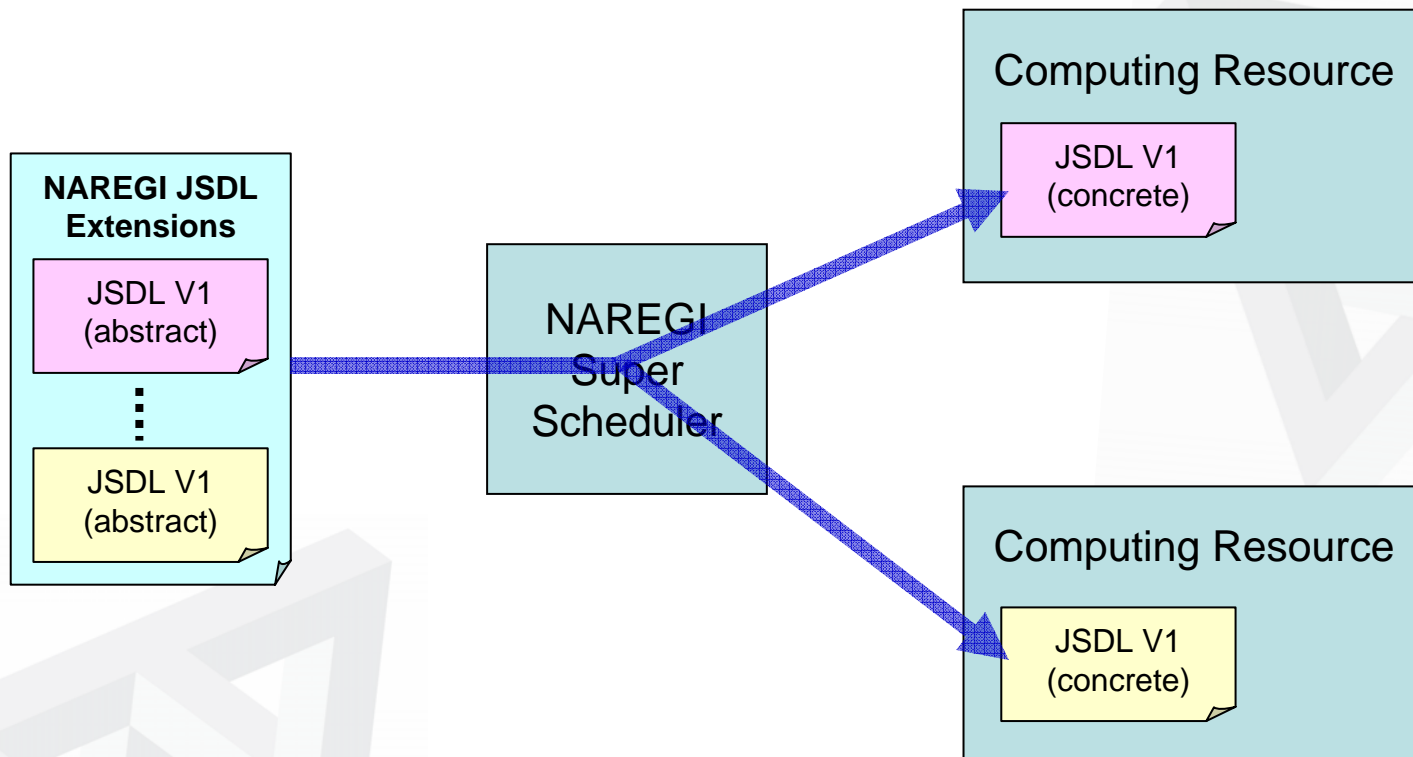
NAREGI Extensions Overview

- Extensions for multiple executables
 - Defined wrapper for multiple JSDL V1 documents



- Extensions for MPI/GridMPI jobs
 - Defined MPI/GridMPI job submission command (e.g. mpirun), and its argument elements

Submission and Execution JSDL



NAREGI JSDL Extensions

- Extensions for Multiple Executables (JSDL V1 wrapper)

```
<naregi:ComplexJobInstance>
```

```
<naregi:JobInstance> ?
```

```
<!-- A JSDL V1 document here -->
```

```
<naregi:AssociateJobID>xsd:string</naregi:AssociateJobID> ?
```

```
</naregi:JobInstance> ?
```

```
<naregi:ComplexJobInstance> <!-- recursive -->
```

```
<!-- JobInstances here -->
```

```
</naregi:ComplexJobInstance>
```

```
</naregi:ComplexJobInstance>
```

not implemented yet

NAREGI JSDL Extensions (Continued)

- Extensions for MPI/GridMPI Job (Application Element)

```
<naregi:MPIApplicationSpecific>
```

```
<naregi:MPIType>xsd:string</naregi:MPIType>
```

```
<naregi:TotalTasks>xsd:positiveInteger<naregi:TotalTasks> ?
```

```
<naregi:TasksPerHost>xsd:positiveInteger<naregi:TasksPerHost> ?
```

```
<naregi:HelperCommand>xsd:string</naregi:HelperCommand> ?
```

```
<naregi:HelperCommandArg>
```

```
  xsd:normalizedString
```

```
</naregi:HelperCommandArg> *
```

```
<!-- ParallelSites -->
```

```
<naregi:AssociateJobs>
```

```
<naregi:AssociateJob>
```

```
<naregi:HostName>xsd:string</naregi:HostName> 1..1
```

```
</naregi:AssociateJob> +
```

```
</naregi:AssociateJobs> ?
```

```
<naregi:MPIApplicationSpecific>
```

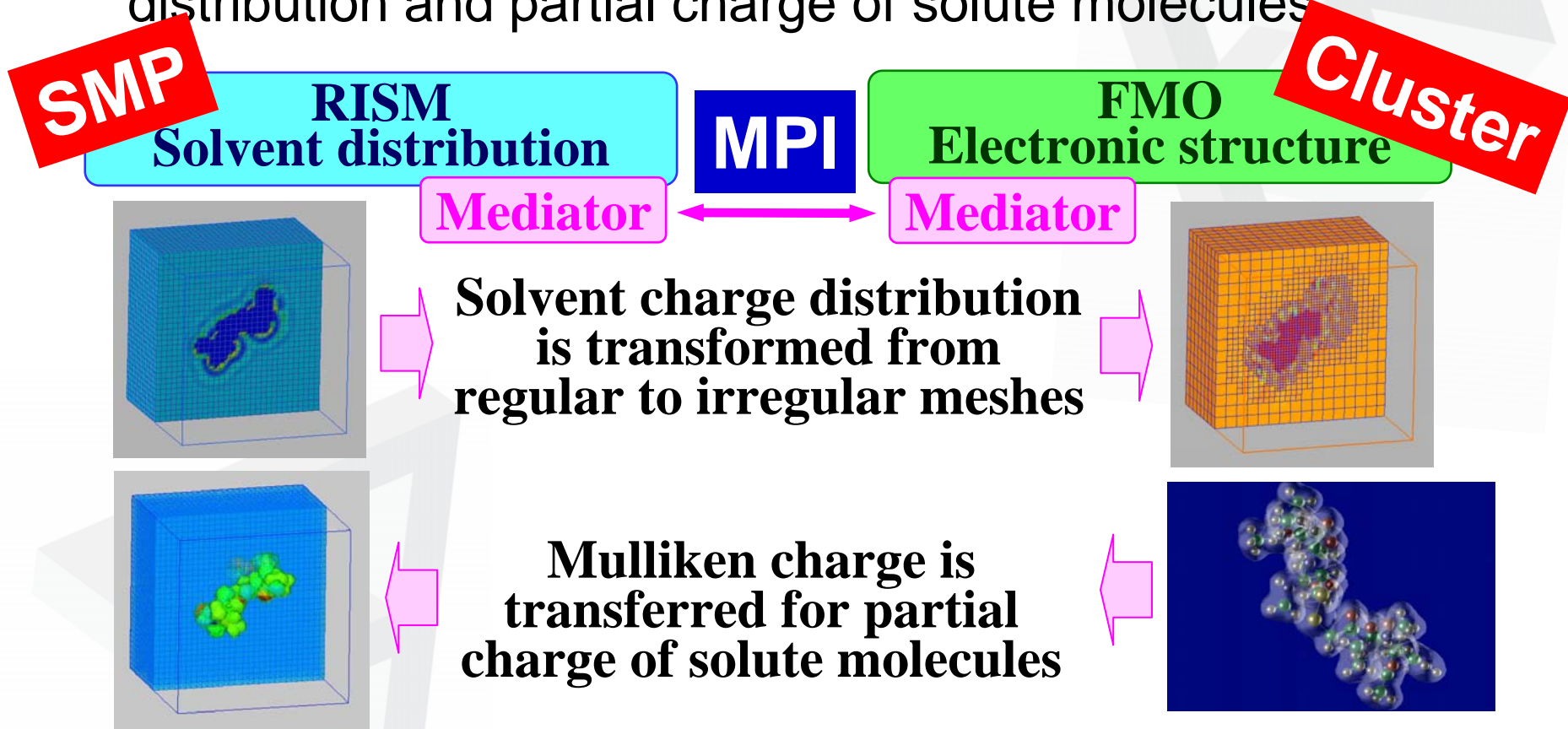
Extended JSDL: Single MPI Job

Refer [FMO](#) example



Co-Allocation Job Use Case: RISM-FMO Coupled simulation

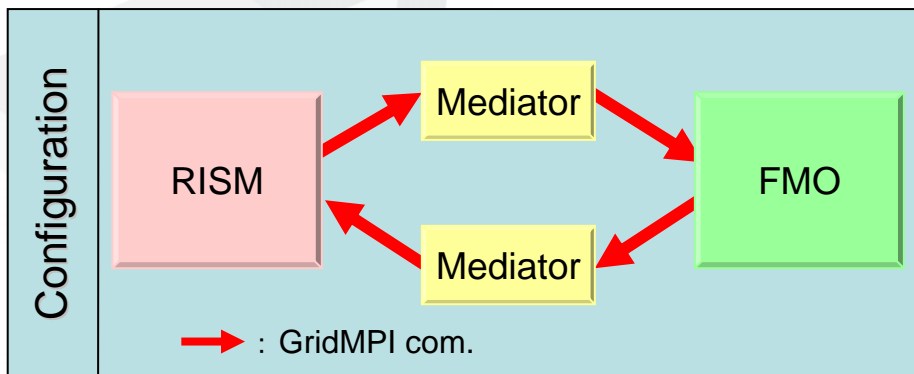
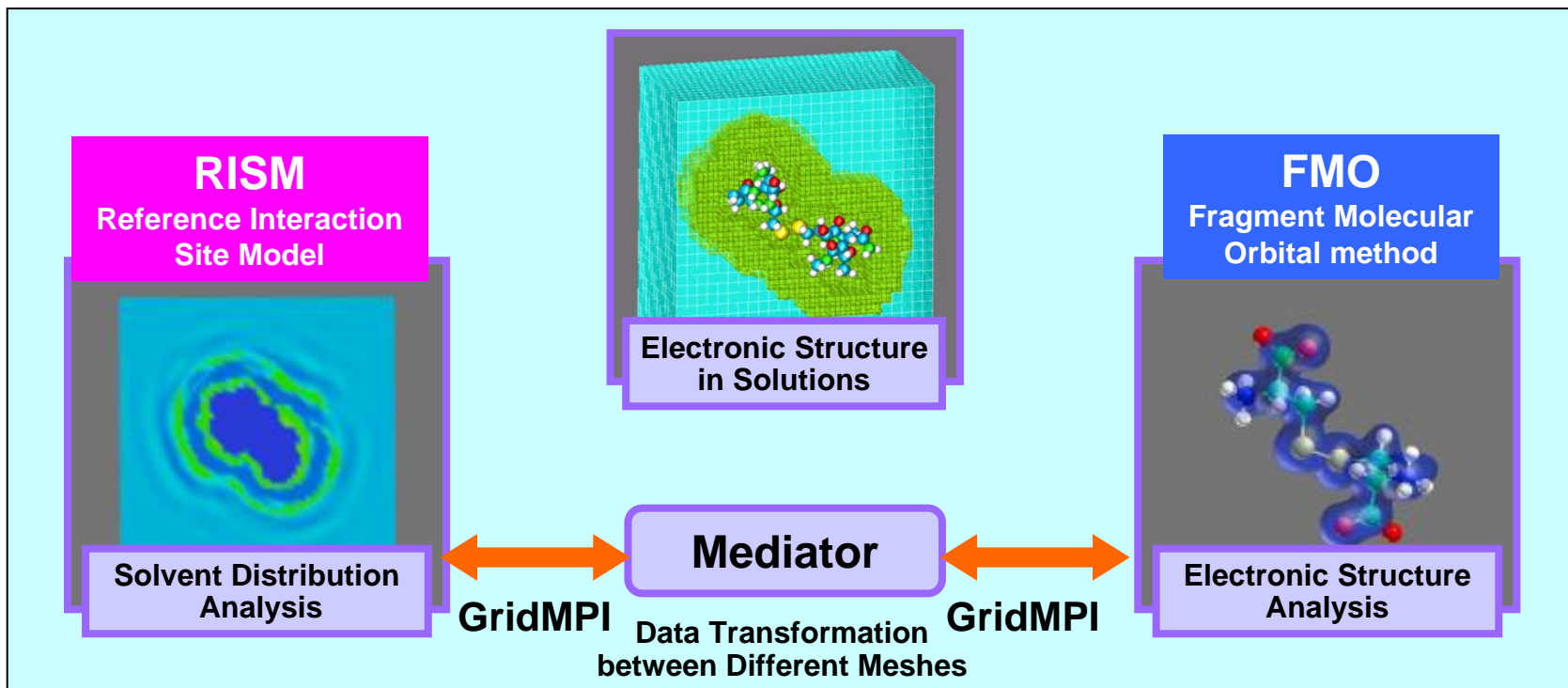
Electronic structure of Nano-scale molecules in solvent is calculated self-consistent by exchanging solvent charge distribution and partial charge of solute molecules



*Original RISM and FMO codes are developed by Institute of Molecular Science and National Institute of Advanced Industrial Science and Technology, respectively.

RISM-FMO Application

A coupled simulation of the electronic structure of a molecule in solution



Requirements

RISM:	CPU=Power4, OS=AIX, #CPUs=32, #nodes=1
FMO:	CPU=Xeon, OS=Linux, #CPUs=10, #nodes=5
Mediator:	CPU=Xeon, OS=Linux, #CPUs=1, #nodes=2

Submission JSDL: RISM-FMO

Refer [RISM-FMO](#) example



Open issues

- There is no way to describe resource requirements between co-allocated job
 - e.g. Network type, bandwidth, latency etc.
- File System Sharing Property
 - Not shared, shared within a cluster, shared within a computing center, shared within a site, shared globally
- Resource description for heterogeneous system configuration in a cluster system
 - There are lot of cases that the nodes in a big cluster system are heterogeneous
 - New nodes addition into a cluster system makes the system heterogeneous
New product has faster CPU, more CPUs (e.g. dual core), bigger memory, bigger disk than the node which installed one years before. Usually users cannot get old product.

Thank you !



FMO Submission JSDL

```
<?xml version="1.0"?>
<JobInstance name="Rfil_gmpi#1_1">
  <JobDocument doctype="http://schemas.ggf.org/jsdl/2005/06/jsdl">
    <JobDefinition xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl"
      xmlns:naregi="http://www.naregi.org/ws/2005/08/jsdl-naregi-draft-02">
      <JobDescription>
        <JobIdentification>
          <JobName>gameSS</JobName>
        </JobIdentification>
        <Application>
          <POSIXApplication
            xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl-posix">
            <Executable>./gameSS</Executable>
            <Output>FMO.out</Output>
            <Error>FMO.err</Error>
            <WorkingDirectory>
              /naregi-beta/home/userdemo/gameSS-2006/gameSS
            </WorkingDirectory>
            <WallTimeLimit>300</WallTimeLimit>
          </POSIXApplication>
          <naregi:MPIApplicationSpecific>
            <naregi:MPIType>GridMPI</naregi:MPIType>
            <naregi:TotalTasks>10</naregi:TotalTasks>
            <naregi:TasksPerHost>2</naregi:TasksPerHost>
          </naregi:MPIApplicationSpecific>
        </Application>
        <Resources>
          <OperatingSystem>
            <OperatingSystemType>
              <OperatingSystemName>LINUX</OperatingSystemName>
            </OperatingSystemType>
          </OperatingSystem>
        </Resources>
      </JobDescription>
    </JobDefinition>
  </JobDocument>
</JobInstance>
```

RISM-FMO Submission JSDL

```
<?xml version="1.0"?>
<ComplexJobInstance xmlns="http://www.naregi.org/ws/ogsa/ems/rss/ces/0.xsd"
  name="Rfil_gmpi#1" type="mpi">
  <JobInstance name="Rfil_gmpi#1_1">
    <JobDocument doctype="http://schemas.ggf.org/jsdl/2005/06/jsdl">
      <JobDefinition xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl"
        xmlns:naregi="http://www.naregi.org/ws/2005/08/jsdl-naregi-draft-02">
        <JobDescription>
          <JobIdentification>
            <JobName>gameess</JobName>
          </JobIdentification>
          <Application>
            <POSIXApplication
              xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl-posix">
              <Executable>./gameess.00.x</Executable>
              <Output>FMO.out</Output>
              <Error>FMO.err</Error>
              <WorkingDirectory>
                /naregi-beta/home/userdemo/rism-gameess-2006/rism-gameess
              </WorkingDirectory>
              <WallTimeLimit>300</WallTimeLimit>
            </POSIXApplication>
            <naregi:MPIApplicationSpecific>
              <naregi:MPIType>GridMPI</naregi:MPIType>
              <naregi:TotalTasks>10</naregi:TotalTasks>
              <naregi:TasksPerHost>2</naregi:TasksPerHost>
            </naregi:MPIApplicationSpecific>
          </Application>
          <Resources>
            <OperatingSystem>
              <OperatingSystemType>
                <OperatingSystemName>LINUX</OperatingSystemName>
              </OperatingSystemType>
            </OperatingSystem>
          </Resources>
        </JobDescription>
      </JobDefinition>
    </JobDocument>
  </JobInstance>
  <JobInstance name="Rfil_gmpi#1_2">
    <JobDocument doctype="http://schemas.ggf.org/jsdl/2005/06/jsdl">
      <JobDefinition xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl"
        xmlns:naregi="http://www.naregi.org/ws/2005/08/jsdl-naregi-draft-02">
        <JobDescription>
          <JobIdentification>
            <JobName>mediator</JobName>
          </JobIdentification>
          <Application>
            <POSIXApplication xmlns="
              http://schemas.ggf.org/jsdl/2005/06/jsdl-posix">
              <Executable>../medocos/bin/mediator</Executable>
              <Output>Mediator.out</Output>
              <Error>Mediator.err</Error>
              <WorkingDirectory>
                /naregi-beta/home/userdemo/rism-gameess-2006/rism-gameess
              </WorkingDirectory>
            </POSIXApplication>
            <naregi:MPIApplicationSpecific>
              <naregi:MPIType>GridMPI</naregi:MPIType>
              <naregi:TotalTasks>2</naregi:TotalTasks>
              <naregi:TasksPerHost>1</naregi:TasksPerHost>
            </naregi:MPIApplicationSpecific>
          </Application>
        </JobDescription>
      </JobDefinition>
    </JobDocument>
  </JobInstance>
</ComplexJobInstance>
```

```

</Application>
<Resources>
  <OperatingSystem>
    <OperatingSystemType>
      <OperatingSystemName>LINUX</OperatingSystemName>
    </OperatingSystemType>
  </OperatingSystem>
  <TotalResourceCount>
    <exact>2</exact>
  </TotalResourceCount>
</Resources>
</JobDescription>
</JobDefinition>
</JobDocument>
</JobInstance>
<JobInstance name="RFile_gmpi#1_3">
  <JobDocument doctype="http://schemas.ggf.org/jsdl/2005/06/jsdl">
    <JobDefinition xmlns="http://schemas.ggf.org/jsdl/2005/06/jsdl"
      xmlns:naregi="http://www.naregi.org/ws/2005/08/jsdl-naregi-draft-02">
      <JobDescription>
        <JobIdentification>
          <JobName>3drism</JobName>
        </JobIdentification>
        <Application>
          <POSIXApplication xmlns=
            "http://schemas.ggf.org/jsdl/2005/06/jsdl-posix">
            <Executable>../rism-gamess.aix/rism/3drism_dex</Executable>
            <Output>RISM.out</Output>
            <Error>RISM.err</Error>
            <WorkingDirectory>
              /naregi-beta/home/userdemo/rism-gamess-2006/rism-gamess
            </WorkingDirectory>
            <Environment name="BASH_ENV">.bashrc</Environment>
            <WallTimeLimit>300</WallTimeLimit>
          </POSIXApplication>
          <naregi:MPIApplicationSpecific>
            <naregi:MPIType>GridMPI</naregi:MPIType>
            <naregi:TotalTasks>1</naregi:TotalTasks>
            <naregi:TasksPerHost>1</naregi:TasksPerHost>
          </naregi:MPIApplicationSpecific>
        </Application>
      </JobDescription>
    </JobDefinition>
  </JobDocument>
</JobInstance>
</ComplexJobInstance>

```