Grid PSE
(Grid Problem Solving Environment)

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Simple & Easy Registration, Deployment and Execution of application programs on Grid environment.

PSE Server: [PSE Toolkit / PSE Application Pool]

Grid Infrastructure (NAREGE Core Middleware)
Scenario for Multi-sites MPI Job Execution

1. Submission
2. Resource discovery
3. Negotiation
4. Reservation
5. IMPI starts
6. MPI job starts
7. MPI init.
8. Visualization
9. Accounting

Application requirement definition

Input files
Output files

Super Scheduler

GridVM
Local Scheduler
IMPI Server

RISM Job
Solute simulation
Different (sub) Jobs

Solvent simulation

Site A
Site B (SMP machine)
Site C (PC cluster)

Co-Allocation

Information Service

Multi-Physics simulation (MPI)

Super Scheduler

PSE

WFT

64 CPUs

128 CPUs

GridMPI

RISM
FMO

Source

Work-flow

…

Co-Allocation

…

Application requirement definition

GridMPI

Different (sub) Jobs

Input files
Output files

Network Communication Interface Process

Super Scheduler

WFT

1: Submission
2: Resource discovery
3: Negotiation
4: Reservation
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Work-flow

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Co-Allocation

…” Multi-Physics simulation (MPI).
Grid PSE Concept

- Provide a framework to distribute user applications on grid
  - Users can register, deploy and retrieve applications by using Grid PSE.
  - Application developers distribute their applications to research communities without a hard task.
  - Application users do not want to care about grid for using application.

- Focus on a legacy application
  - Deploy application binaries for specific targets
  - Compile from source program, if needed
Usage I (Registration, Compilation and Deployment)

Application Developer

Enter Application Info.

Upload files
- Source programs
- Compile script etc.

Compile

Grid PSE

Application Pool

Application files

Deployment Info.

Resource Info.

Info. Service

Server#1

Compile OK!

Server#2

Post process NG!

Server#3

Post process OK!

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Registration, Compilation and Deployment

- **Registration**
  1. Upload files (e.g., source code/executables, compile script, post-process script, initial input files, etc.) to the PSE application pool
  2. Upload information (e.g., description, system requirements, etc.) associated with the uploading application to the application pool

- **Compilation (if needed)**
  1. Select an application and a server for compilation
  2. PSE transfers necessary files (e.g., source code) from the application pool to the compile server
  3. PSE compiles and verifies them on the server
  4. PSE transfers files (e.g., executable) from the server to the application pool

- **Deployment**
  1. Select an application and servers that meet the system requirements for application deployment
  2. PSE transfers the executable in the application pool to the selected servers
  3. (Optional) Execute a post-process defined by user to configure and/or verify deployment on each servers
  4. PSE registers information on the deployed servers to the information service
Usage II (Retrieval and Execution)

Application

User

Compose WF

WF execution request (job submission)

Execute on the suitable resource

WFT

Retrieve Application

Application Info.

Grid PSE

Application Info.

• System Requirements etc.

Resource Info.

Info. Service

Server#1

Deployed

Load: high

Server#2

Not deployed

Load: low

Server#3

Deployed

Load: low

Compose WF

Workflow execution request (job submission)

Execute on the suitable resource

Super Scheduler

Retrieve Application

Application Info.

Resource Info.

Info. Service

Grid PSE

Application Info.

• System Requirements etc.

Deployed

Load: high

Server#1

Not deployed

Load: low

Server#2

Deployed

Load: low

Server#3

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Retrieval and Execution

Application Retrieval
1. Retrieve application using GUI
2. Import the information of selected application (system requirements - JSDL, etc.) from application pool to workflow icon of Workflow Tool (WFT)

Execution
1. Compose a workflow job from the registered workflow icon
2. WFT submits a job to Super-Scheduler
3. Super-Scheduler dispatches resource referring the resource information provided by Information Service
Grid PSE Configuration

Grid PSE

Register-UI

Deploy-UI

Application Pool

Deployment Service

compile

deploy

un-deploy

Client

NAREGI WFT

NAREGI IS

NAREGI SS

Register application info.

Register deploy info.

Deploy

Submit

Contents (WF)

Application Information

EPR

GetContent

Request to deploy

Register

AA File
Grid PSE (Summary)

- Grid PSE provides a framework to distribute user applications on the grid.
- Grid PSE enables users
  - to register their own applications,
  - to compile and deploy the applications in the grid,
  - to retrieve the application information,
  - and to export it to WFT as a program icon for execution.
- “Application Pool” of Grid PSE is based upon ACS specification discussed in GGF ACS-WG.