PHOSPHORUS

Rapid Deployment of VS Workflows on PHOSPHORUS using Meta Scheduling Service

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Outline

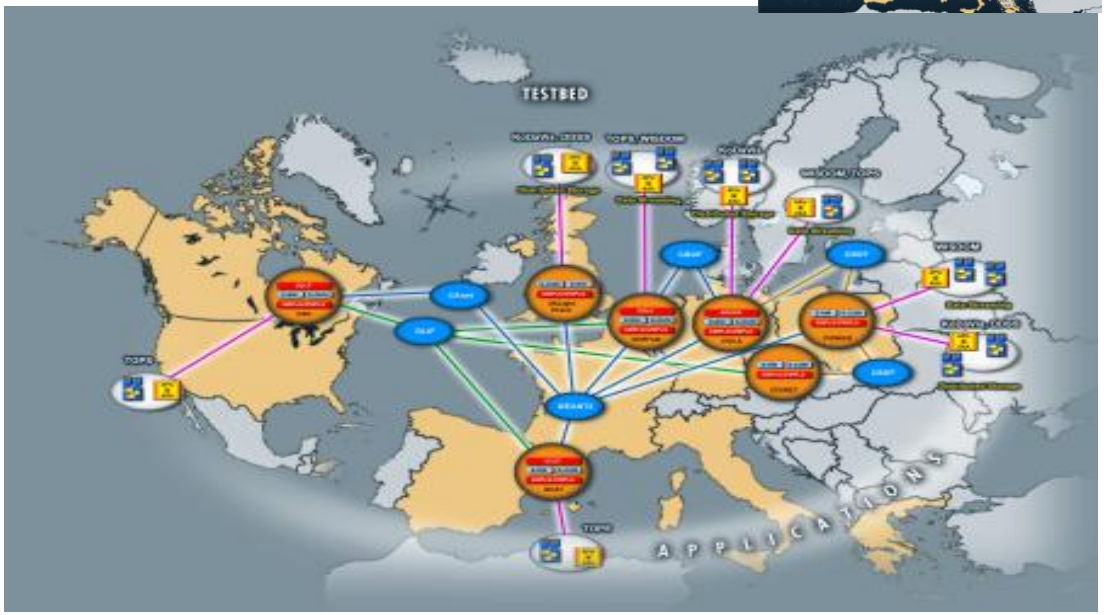
- Introduction and Motivation
  - Bioinformatics Applications on the Grid
  - PHOSPHORUS Testbed
  - Objectives within PHOSPHORUS
- Issues related to Grid VS deployment
- Development of a VS Framework in PHOSPHORUS
  - Virtual Screening Applications
  - vHTS Framework Design
- High throughput Virtual Screening Workflows
- Conclusions
- Example VS Deployment using UNICORE/MSS

Biomedical/Bioinformatics Applications

- High computational and data storage demands
- Data security/privacy restrictions
- High Throughput data management & deployment on large-scale Grids
- Need of high level tools to enable e-Scientists to use Grids in an easy and transparent way

PHOSPHORUS Testbed

- Large capacity optical networks
- Satisfying e-Science HPC applications' (high computational & networking) demands…
- Needed: Advanced Grid-aware tools



Objectives within PHOSPHORUS

- Rapid deployment of VS applications to PHOSPHORUS environment
- Using user-friendly workflows based on UNICORE6 / MSS integration
- Efficient Stage-in and stage-out: easy distribution of input and output data
- Data distribution and collection without any data loss
- Support for post-processing and analyses

Issues in using Large-scale Grids

- Management and deployment of large number of jobs
- Scheduling policy: maximum resource utilization in the available time and space
- Pre/Post processing, management of huge amount of output data
- The production environment should provide automated and fault tolerant jobs and files management

Issues in using Large-scale Grids II

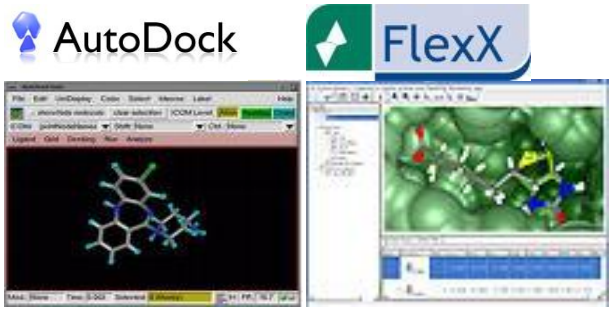
- The amount of transferred data impacts on the overall Grid performance
- Efficient Data distribution on the Grid storage
- Speedy transfer between computing elements and Grid storage.
- Automated post processing: data mining

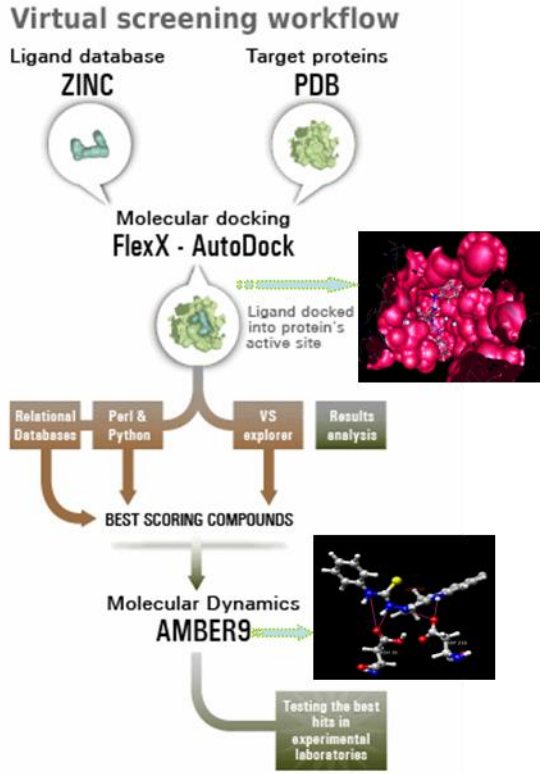
Development of a VS Framework

- Support large-scale deployment of virtual screening services in PHOSPHORUS
- Addressing the issues involved in deployment of complex VS workflows
- An extensible framework making the Grid more accessible to end users

Virtual Screening by Molecular Docking

- CPU and Data intensive applications:
- FlexX (BioSolveIT)
  - Predicts geometry/binding free energy of protein ligand complex
- AutoDock (Scripps Research Institute)
  - Comparatively time-consuming, a single docking job takes ~ 30-60 minutes on a standard CPU.
- Amber (MD Simulations)
  - Package for simulations of biomolecules.
- INPUT/OUTPUT data:
  - Several GB to TB.





High Throughput VS Framework

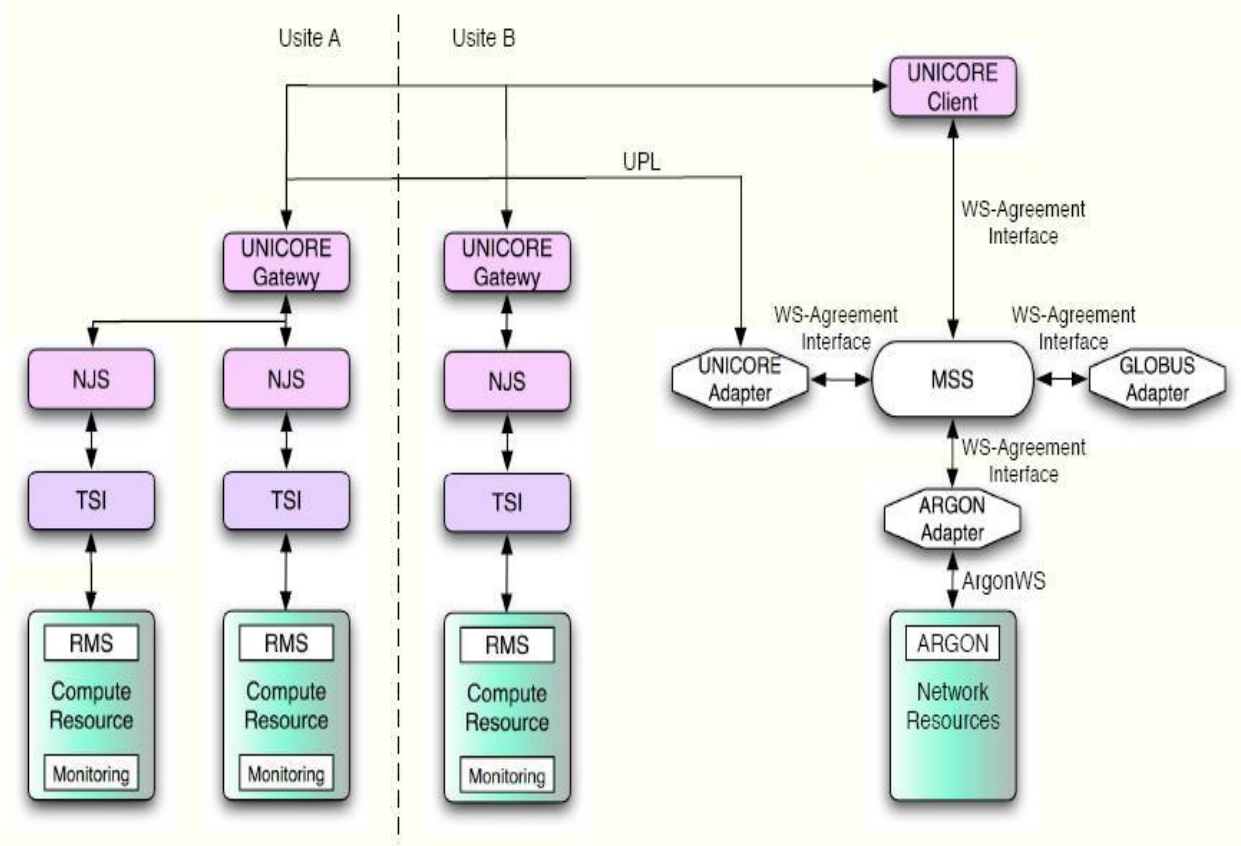
- Using UNICORE-6 Middleware Technology
  - Seamless, secure and transparent access to Grid
  - Ease of use, reduced complexity, increased security
- Using UNICORE Client extensions/plugins
  - Simplifying interactions with applications on the Grid
- Using Meta Scheduling Service
  - Further support to utilize Grid resources

UNICORE Client Extension

- UNICORE Expert Client uses eclipse RCP mechanism
- RCP is based on plug-in architecture that provides development of extendible components
- UNICORE Client: communication to UNICORE services
- The client extension provides interface to the Meta Scheduling Service
- Exploits job/data management mechanism of UNICORE client

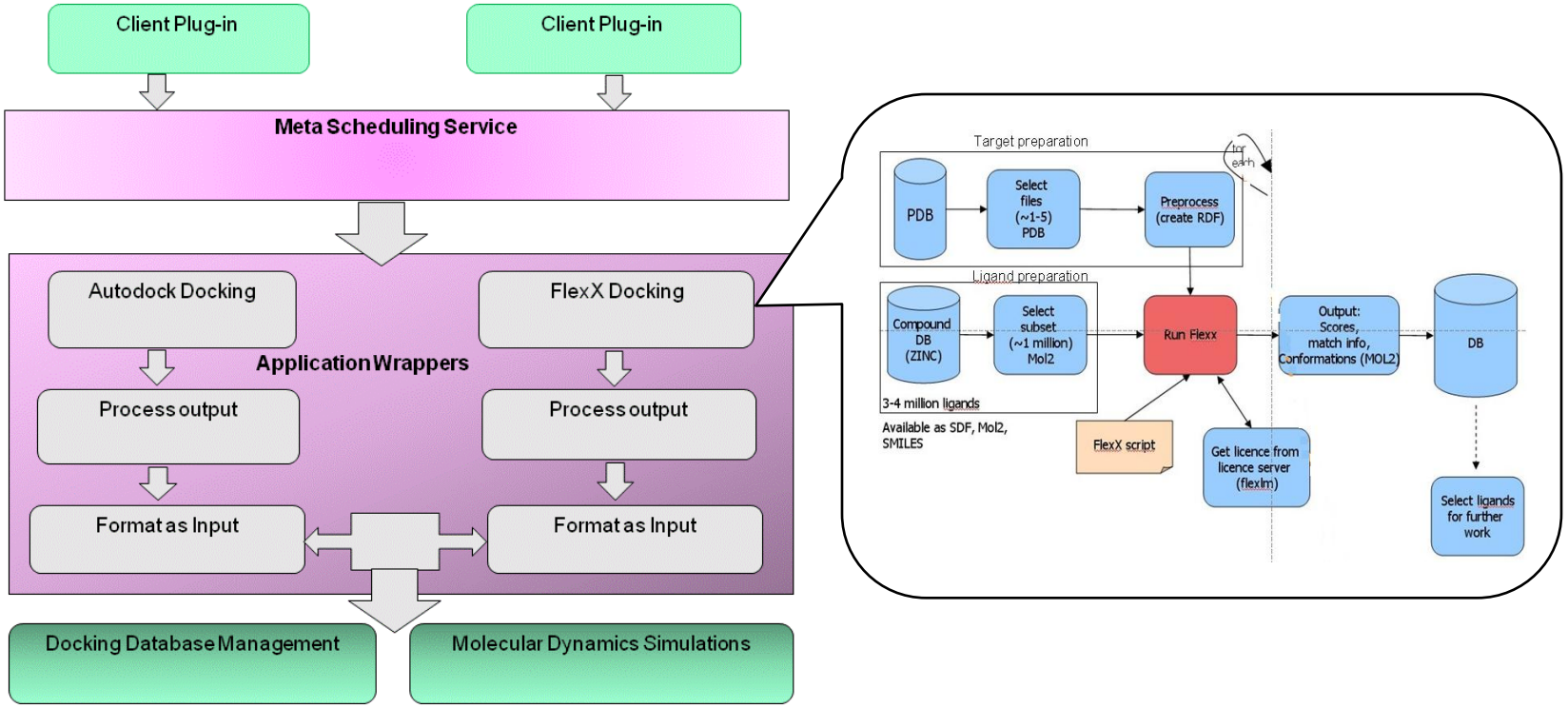
Meta Scheduling Service

- Orchestration & co-ordination of Grid resources, SLA
- Supporting users to utilize maximum available resources
- Workload distribution...



High Throughput Virtual Screening Workflow

- VS Applications: FlexX, AutoDock...
- Fully automated workflow

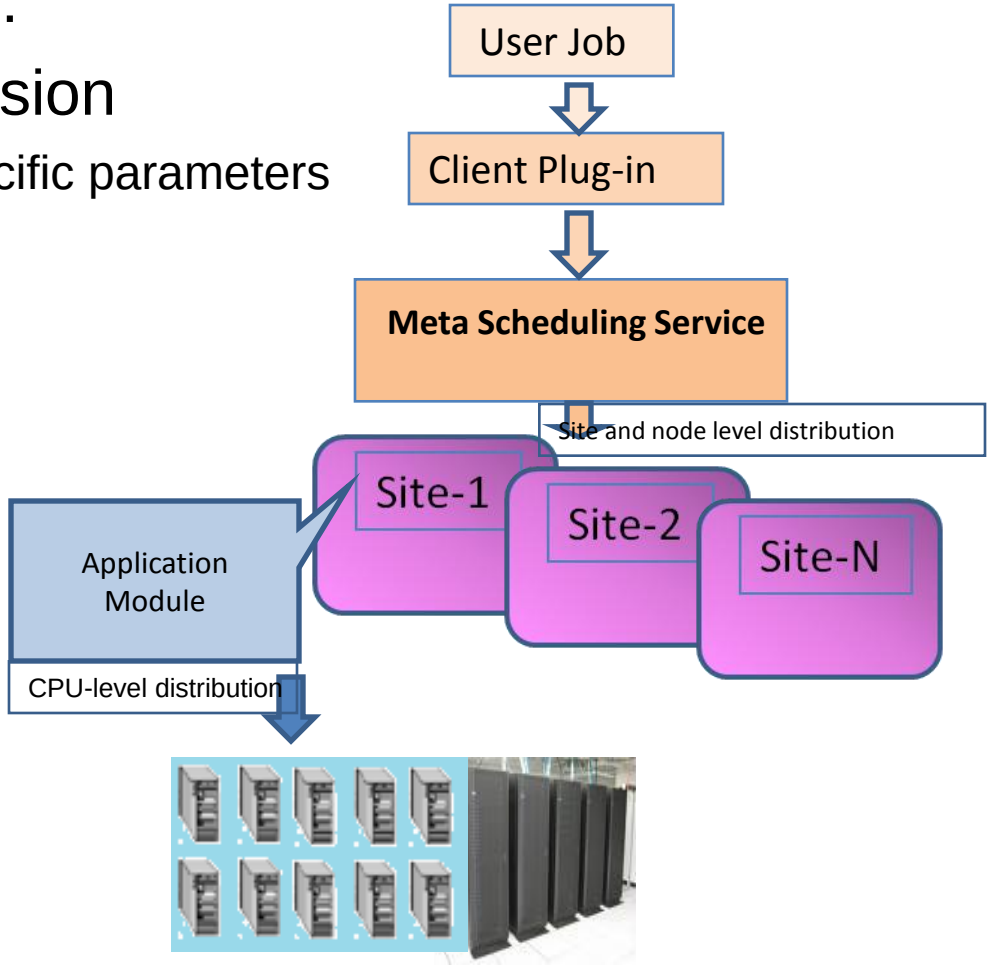


High Throughput Virtual Screening Workflow

Example VS Workflow:

One single job submission

- Setting up Application specific parameters
- Input/output specification

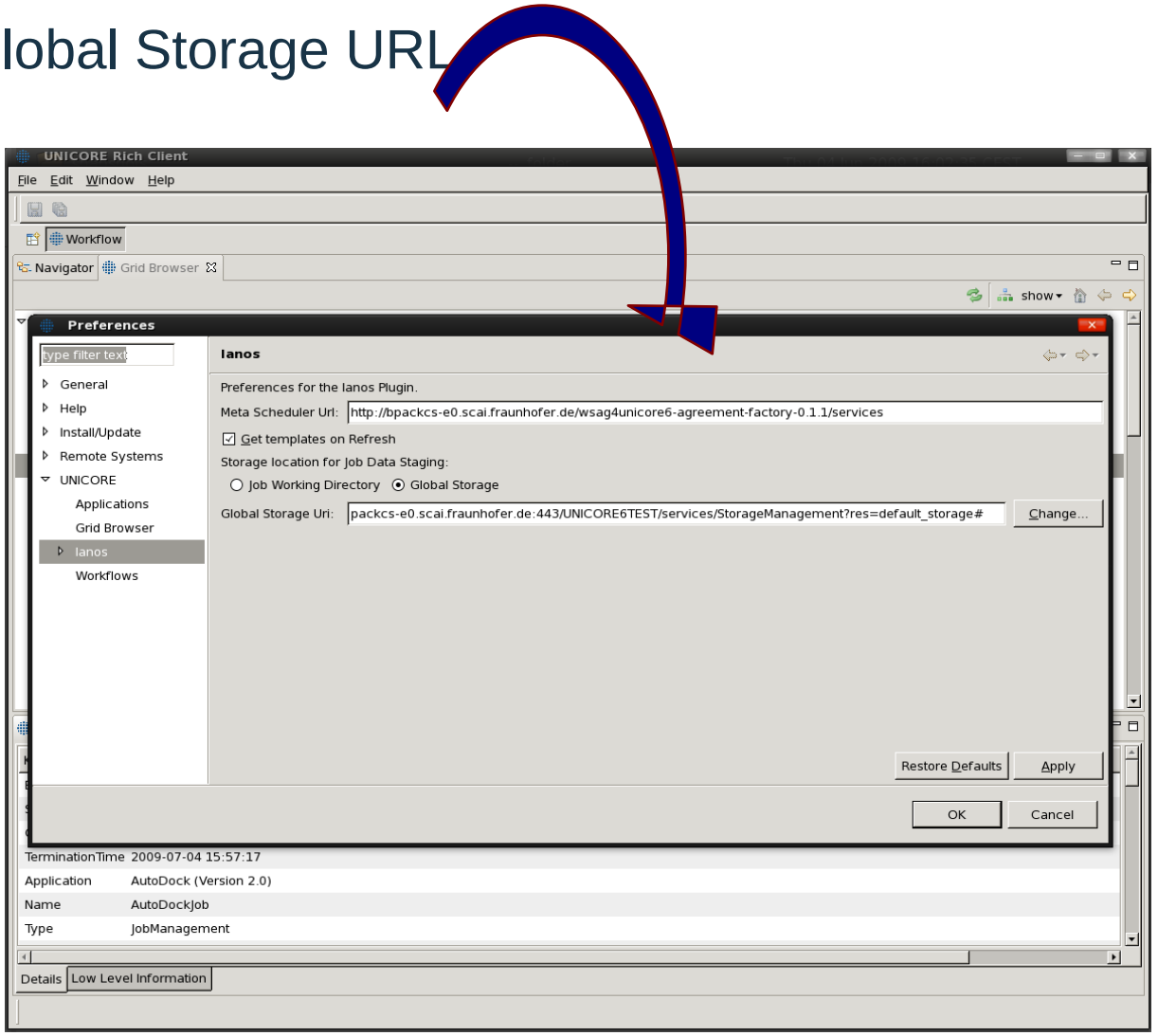


Conclusions

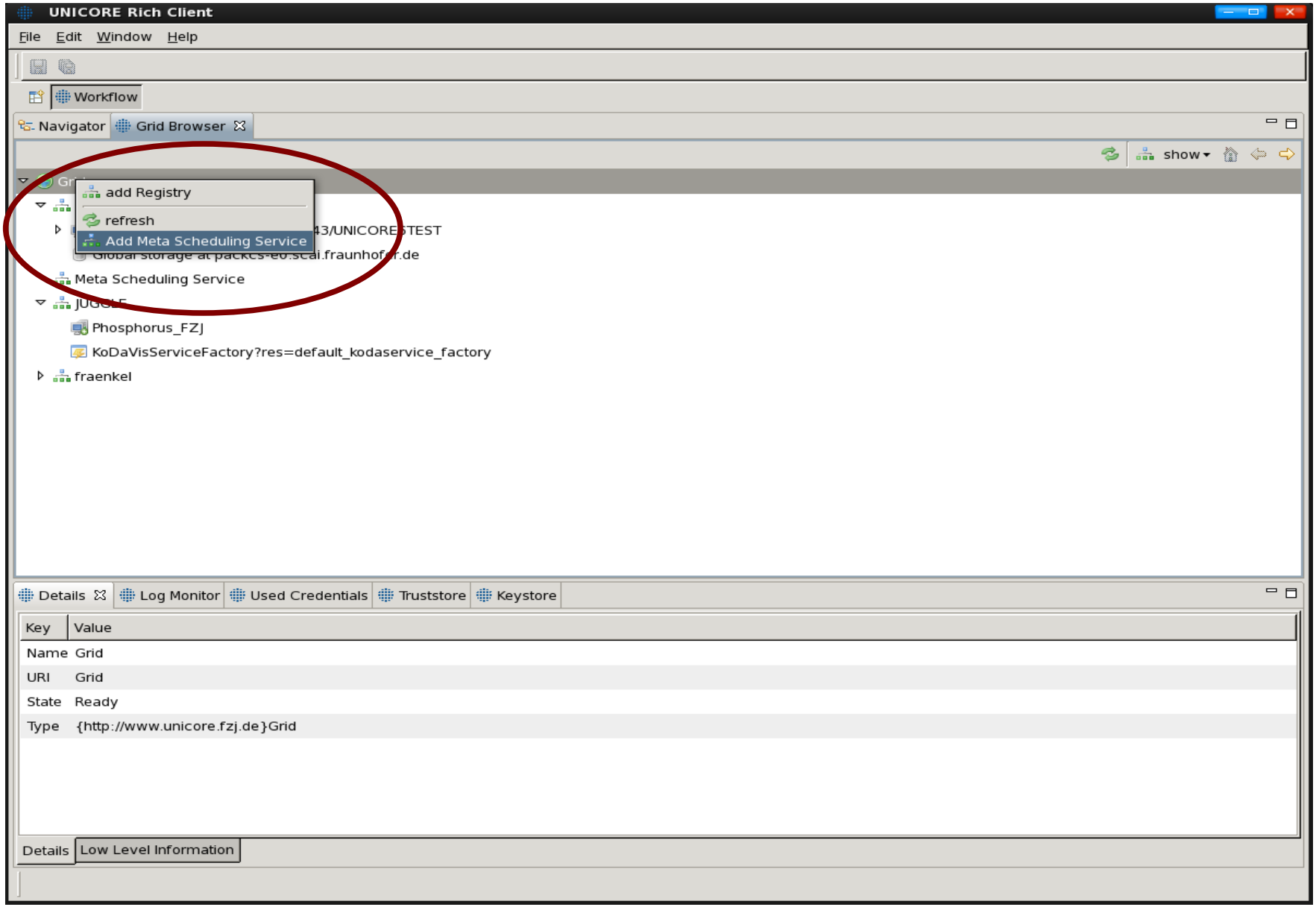
- Rapid deployment
  - High bandwidth input/output (PHOSPHORUS network layer)
- Better deployment efficiency with MSS than using UNICORE client plug-ins alone
- Simplifies, speeds up the complex virtual screening process in the Grid environment
- Flexibility and extensibility
- Allow easy integration of other tools & services

Example VS Deployment: UNICORE/MSS (1/9)

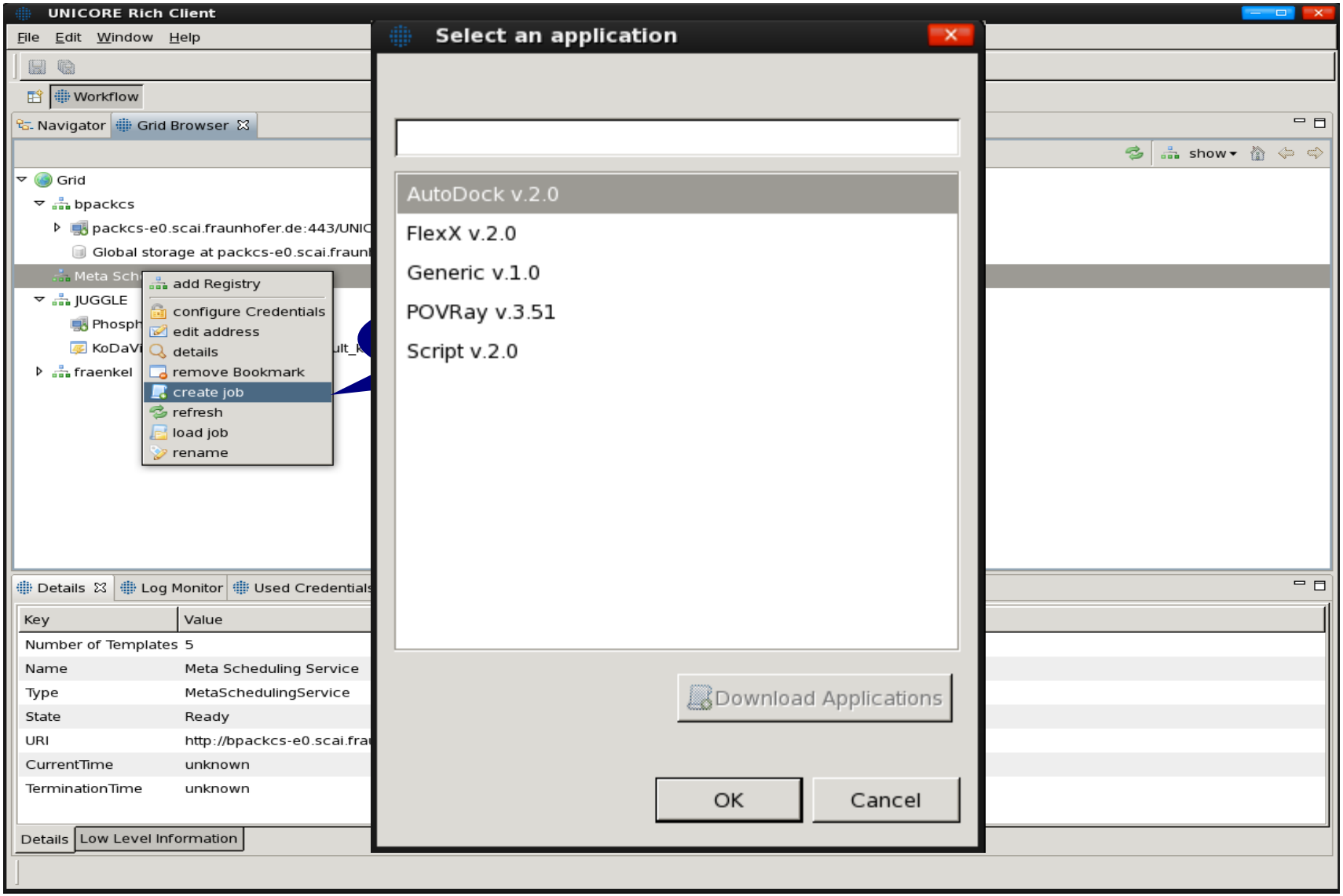
- Load MSS Client Plugin
- Provide MSS URL, Global Storage URL
  - Input/Output



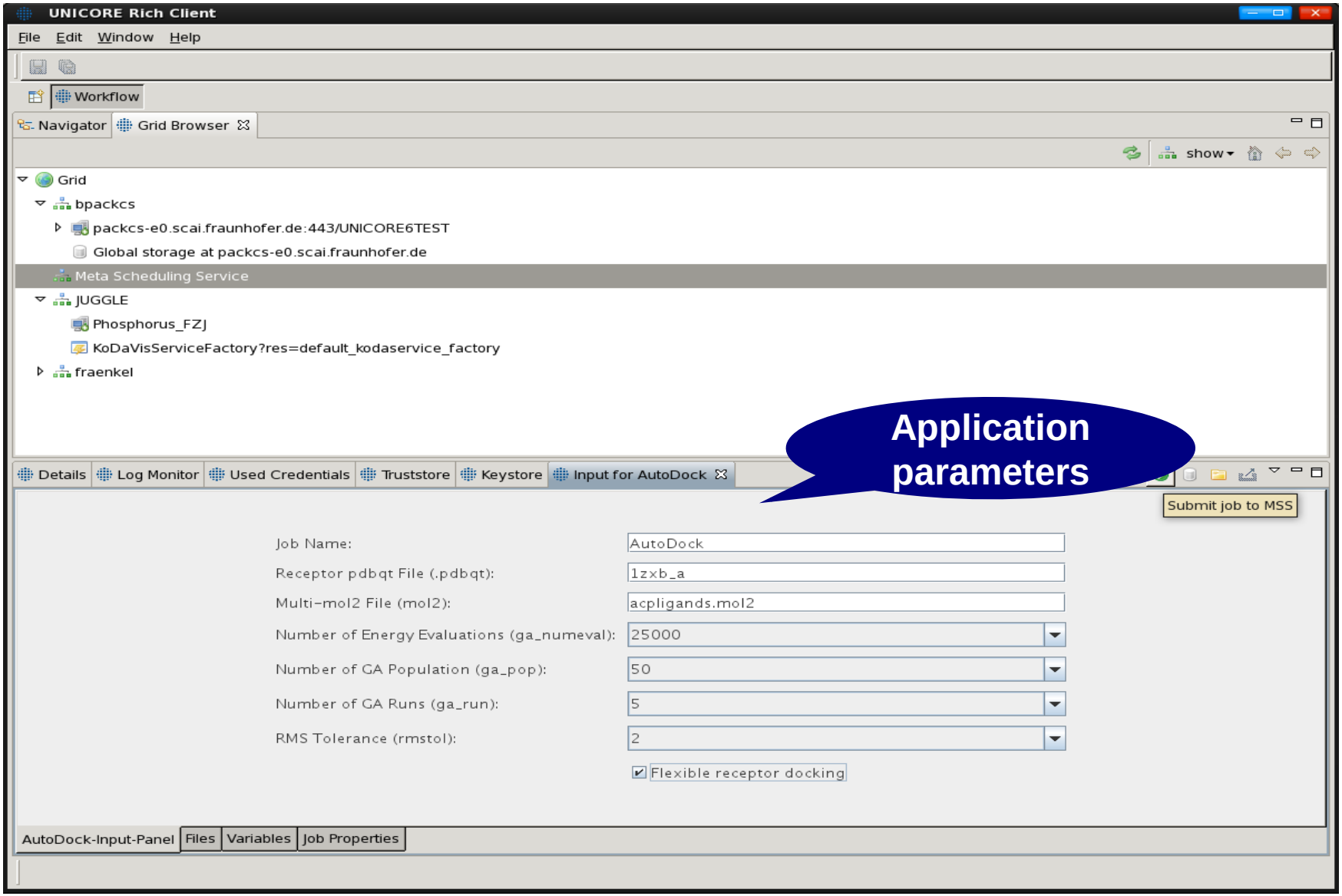
Example VS Deployment: UNICORE/MSS (2/9)



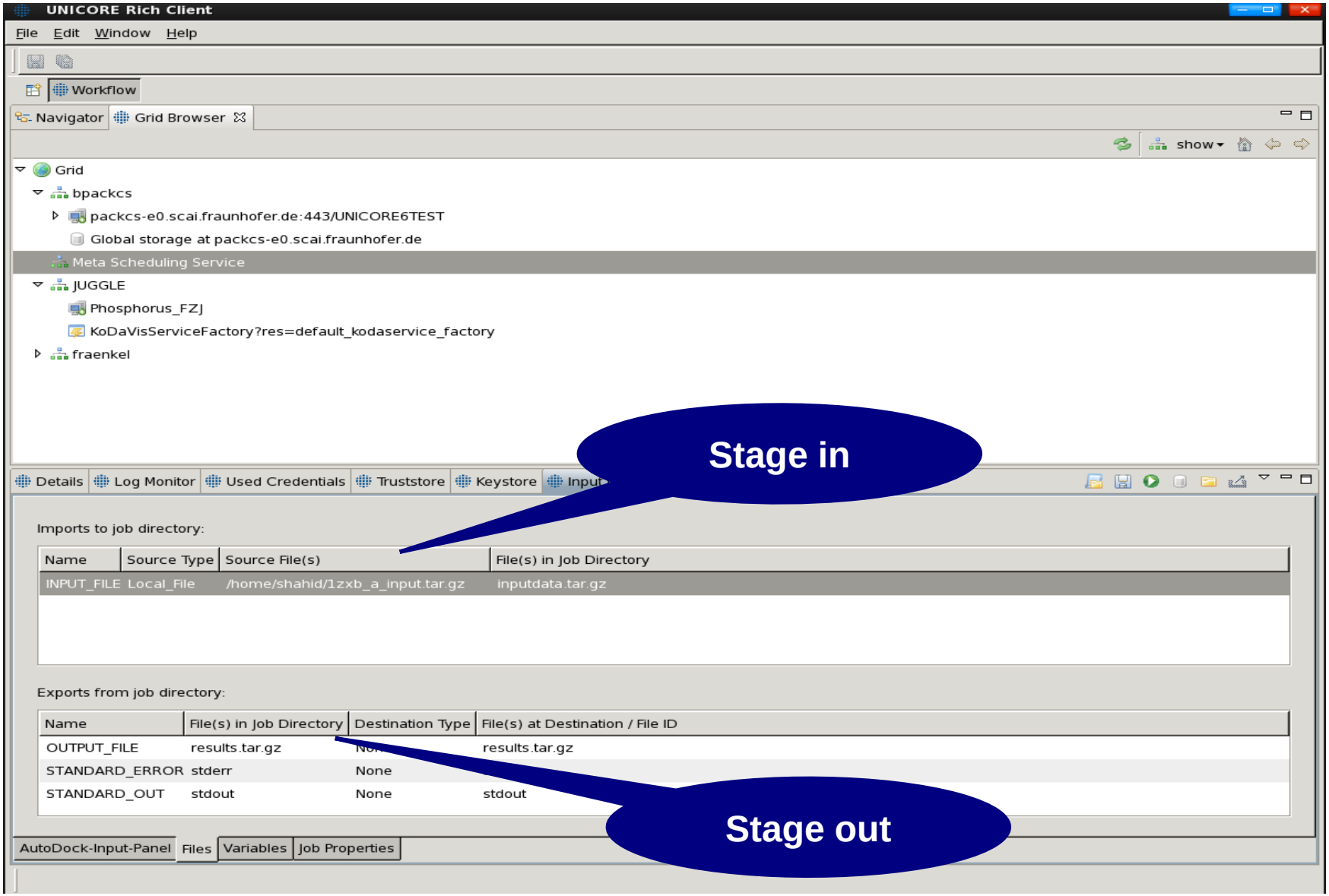
Example VS Deployment: UNICORE/MSS (3/9)



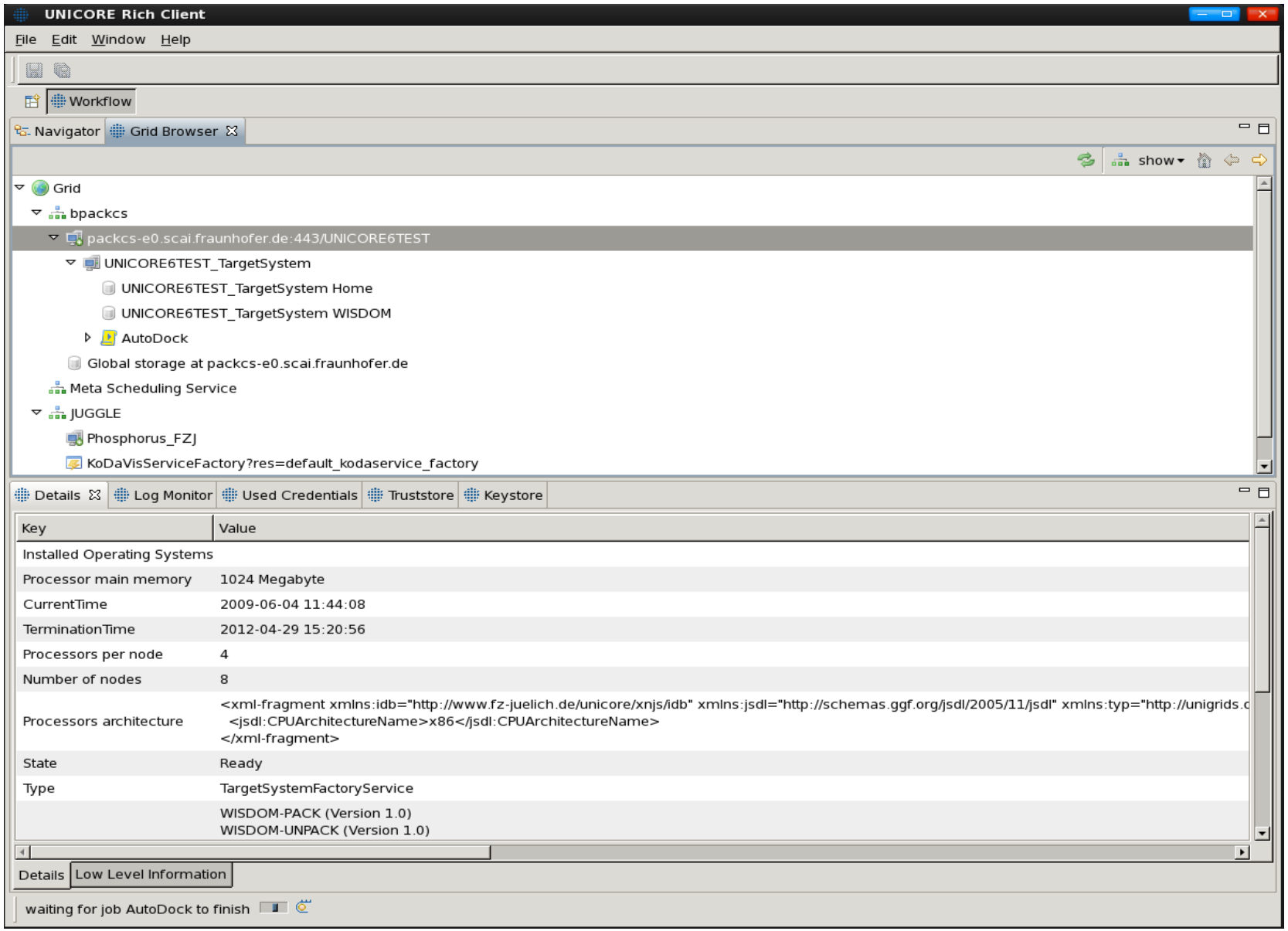
Example VS Deployment: UNICORE/MSS (4/9)



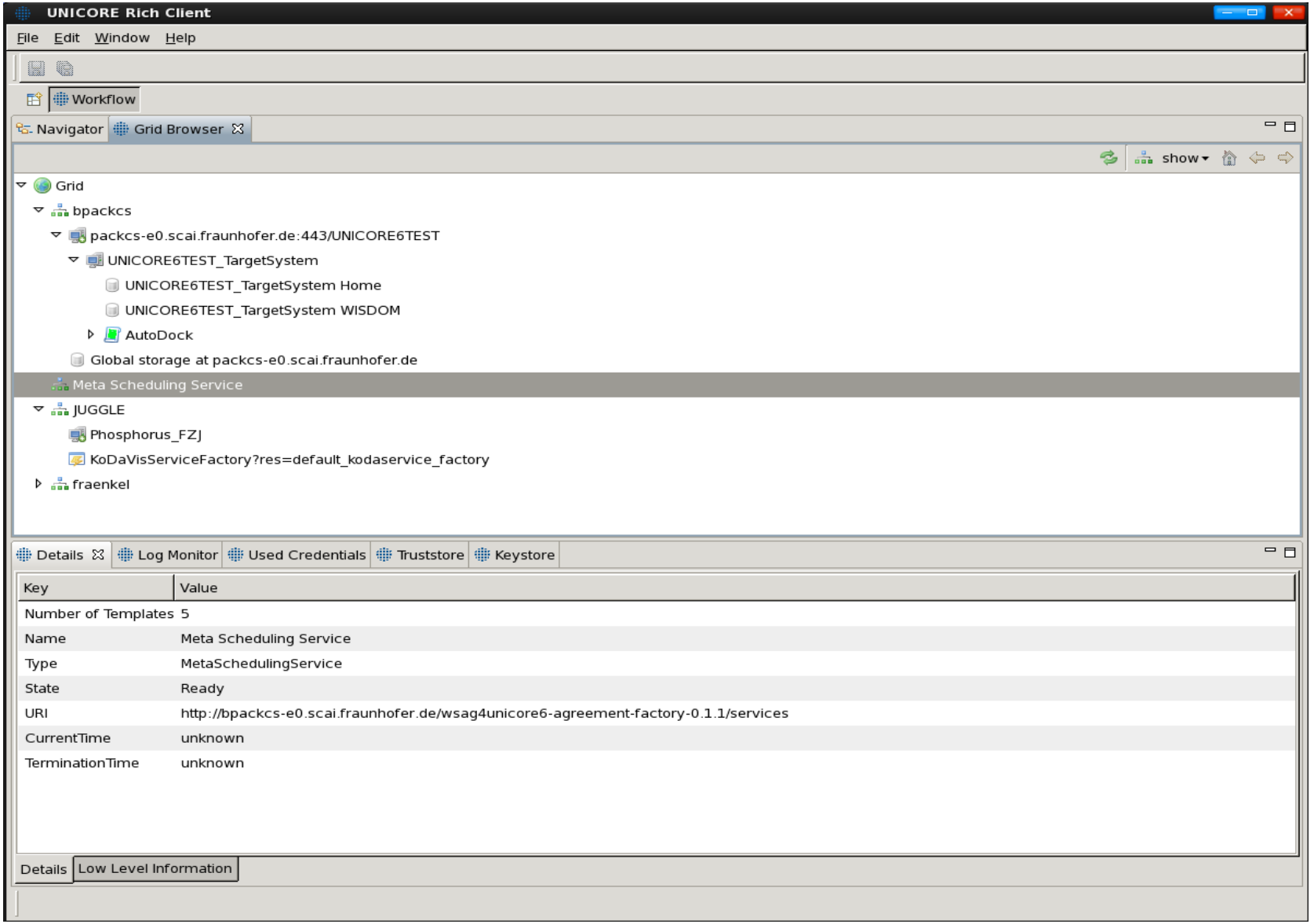
Example VS Deployment: UNICORE/MSS (5/9)



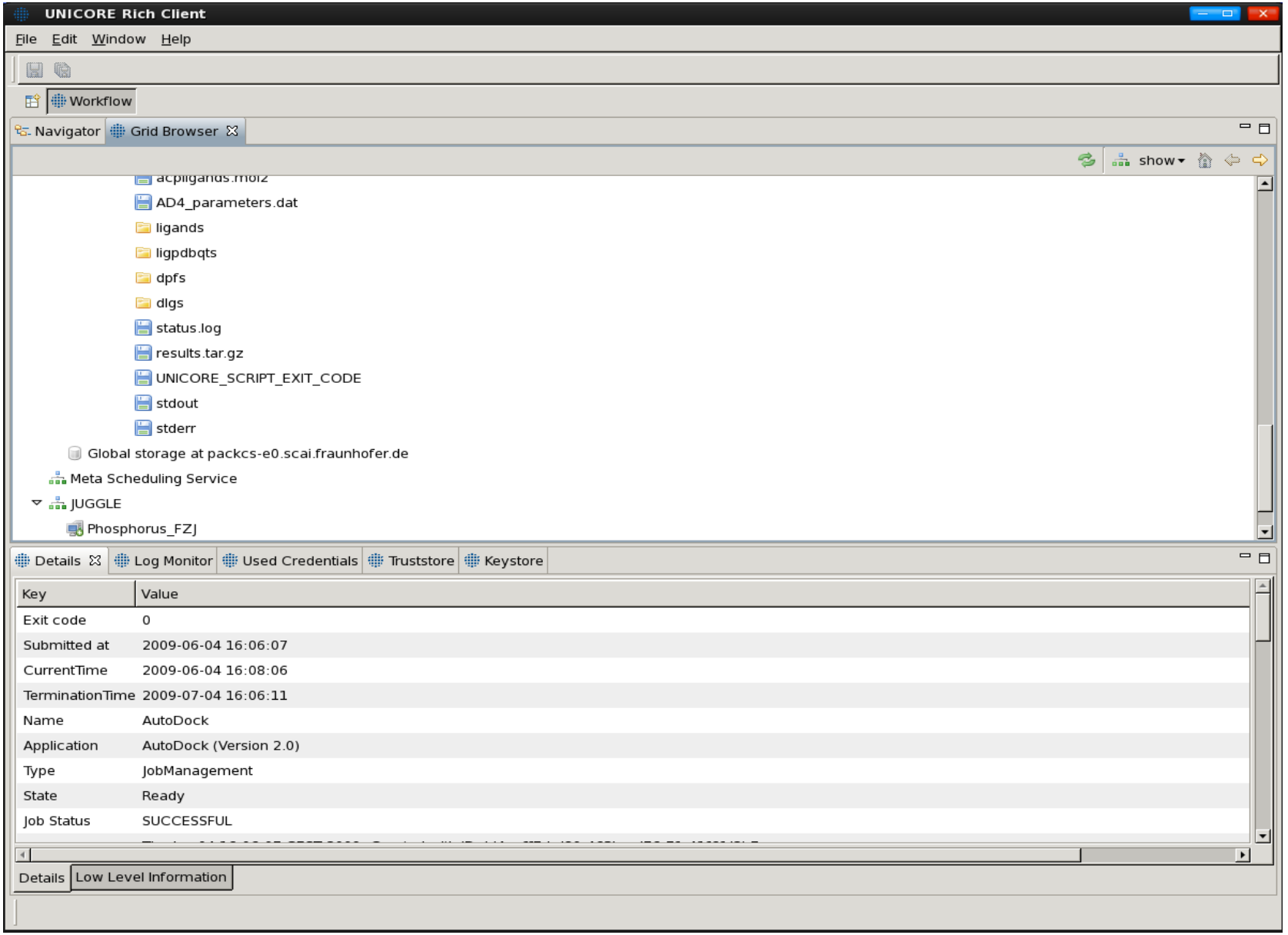
Example VS Deployment: UNICORE/MSS (6/9)



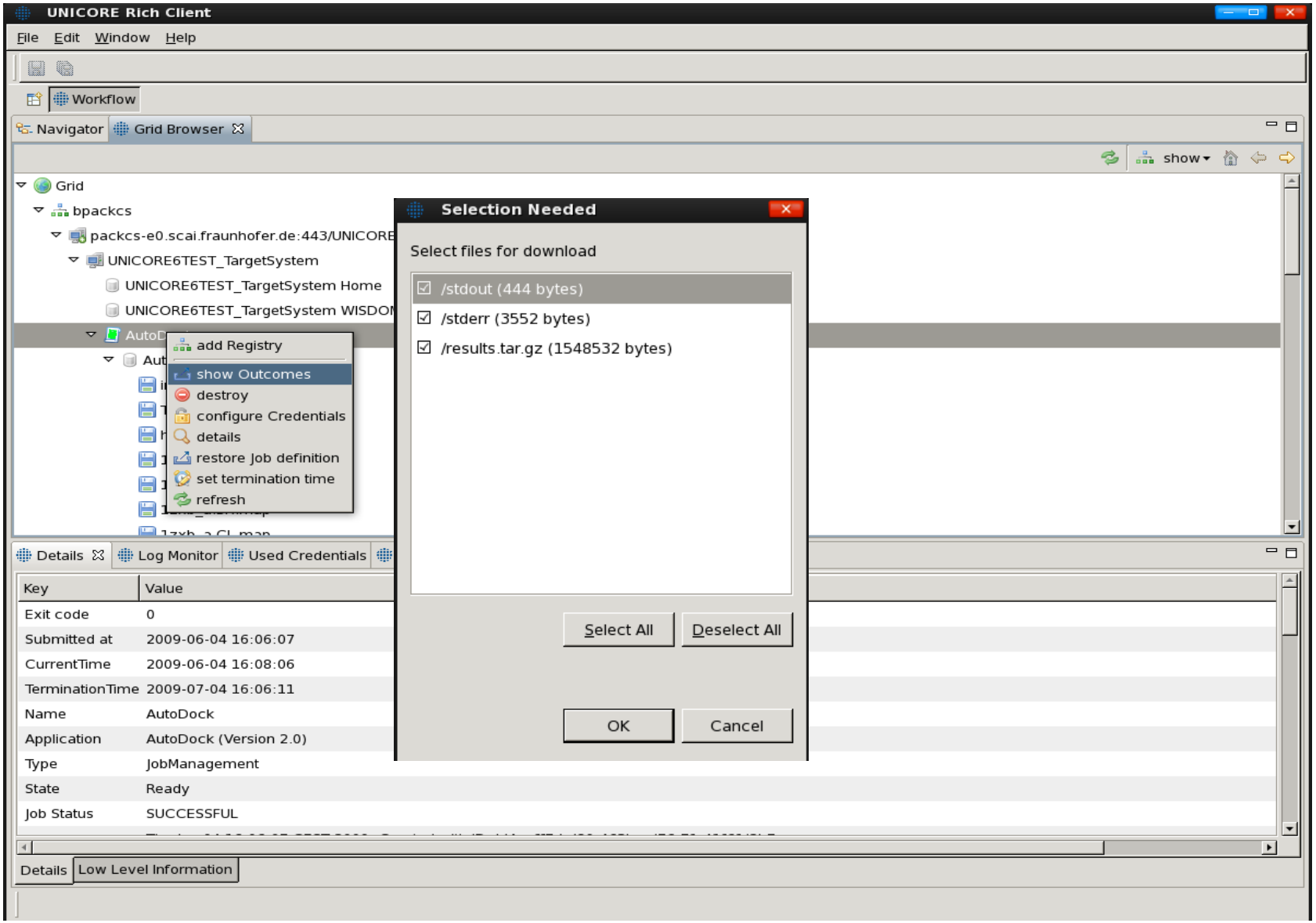
Example VS Deployment: UNICORE/MSS (7/9)



Example VS Deployment: UNICORE/MSS (8/9)



Example VS Deployment: UNICORE/MSS (9/9)



Example VS Deployment

Thank You for your attention