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Enhancing the performance of scientific workflow execution in e-Science environments by harnessing the standards based Parameter Sweep Model

23. July 2013 | **Shahbaz Memon**, Sonja Holl, Bernd Schuller, Andrew Grimshaw

Outline

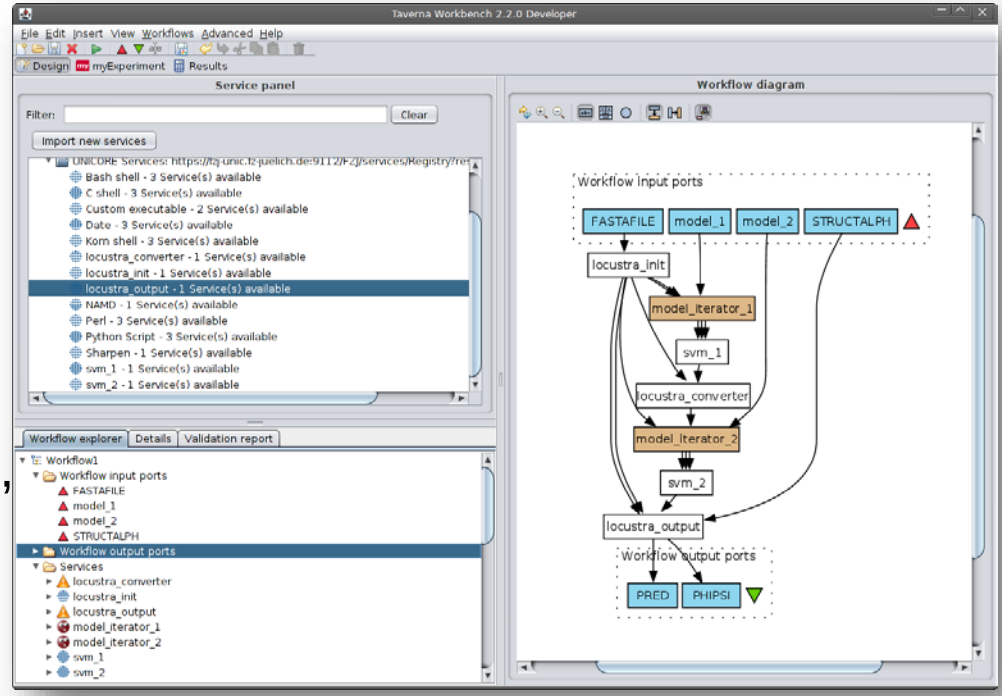
- Introduction
- Taverna Workflow System
- UNICORE
- Motivation: Advanced Workflow Optimization
- JSDL-Parameter Sweep
- UNICORE Parameter Sweep Implementation
- Conclusions

Introduction

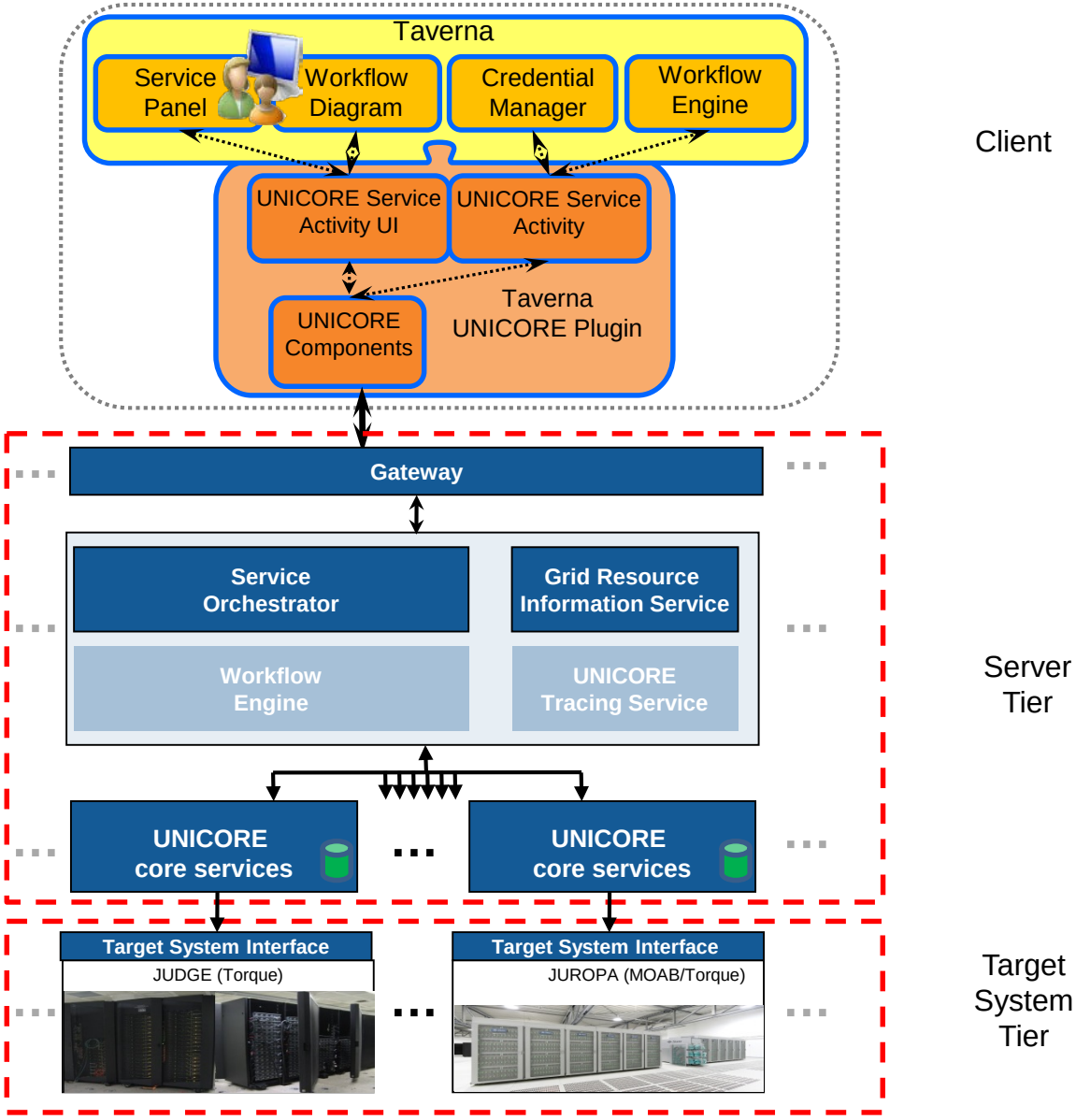
- Scientific workflows are extensively being used for defining and generating computer simulations
- Same application need rerun with different parameters – e.g. verifying and validating simulation models
- Parameter sweep concept can be used to represent an abstract job with iterative parameters
- An improved workflow optimization use case through the use of parameter sweep concept
- UNICORE is used as a Job submission and management middleware

Taverna Workflow System

- Open source written in Java
- Graphical Interface: Workbench
- Execution: Taverna Worfklow Engine
- Data Flow Driven
- Activities represent Web services, Java classes, local scripts
- UNICORE plugin was developed in 2010

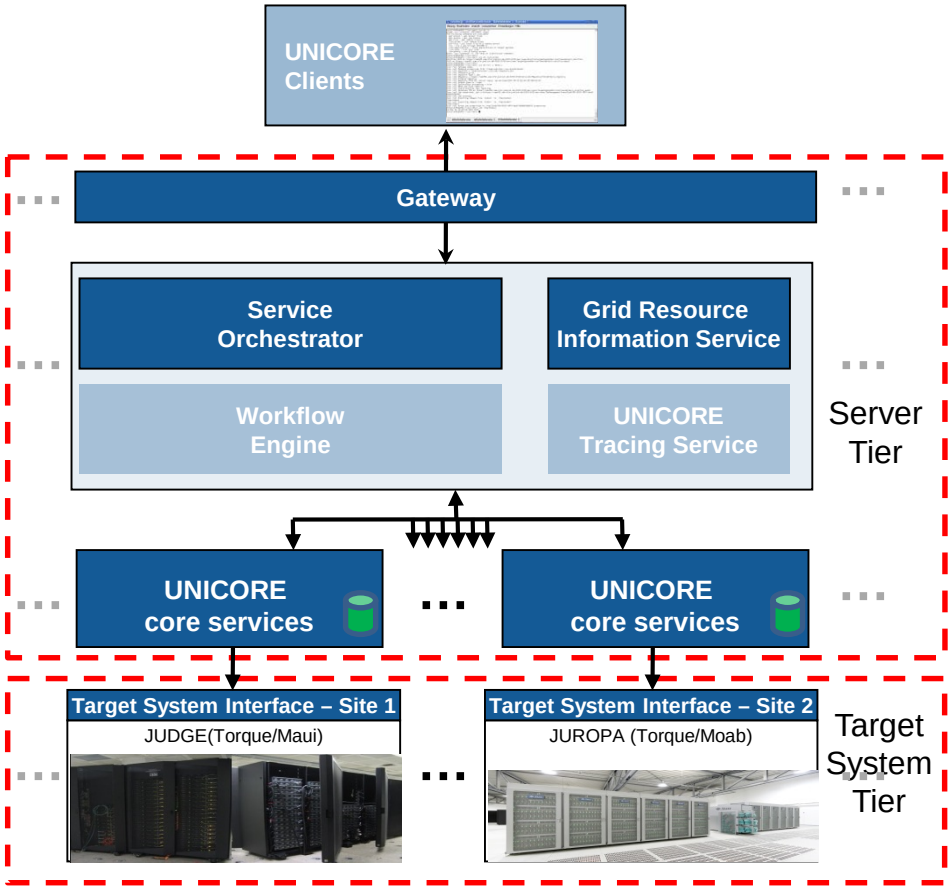


Integrated Architecture



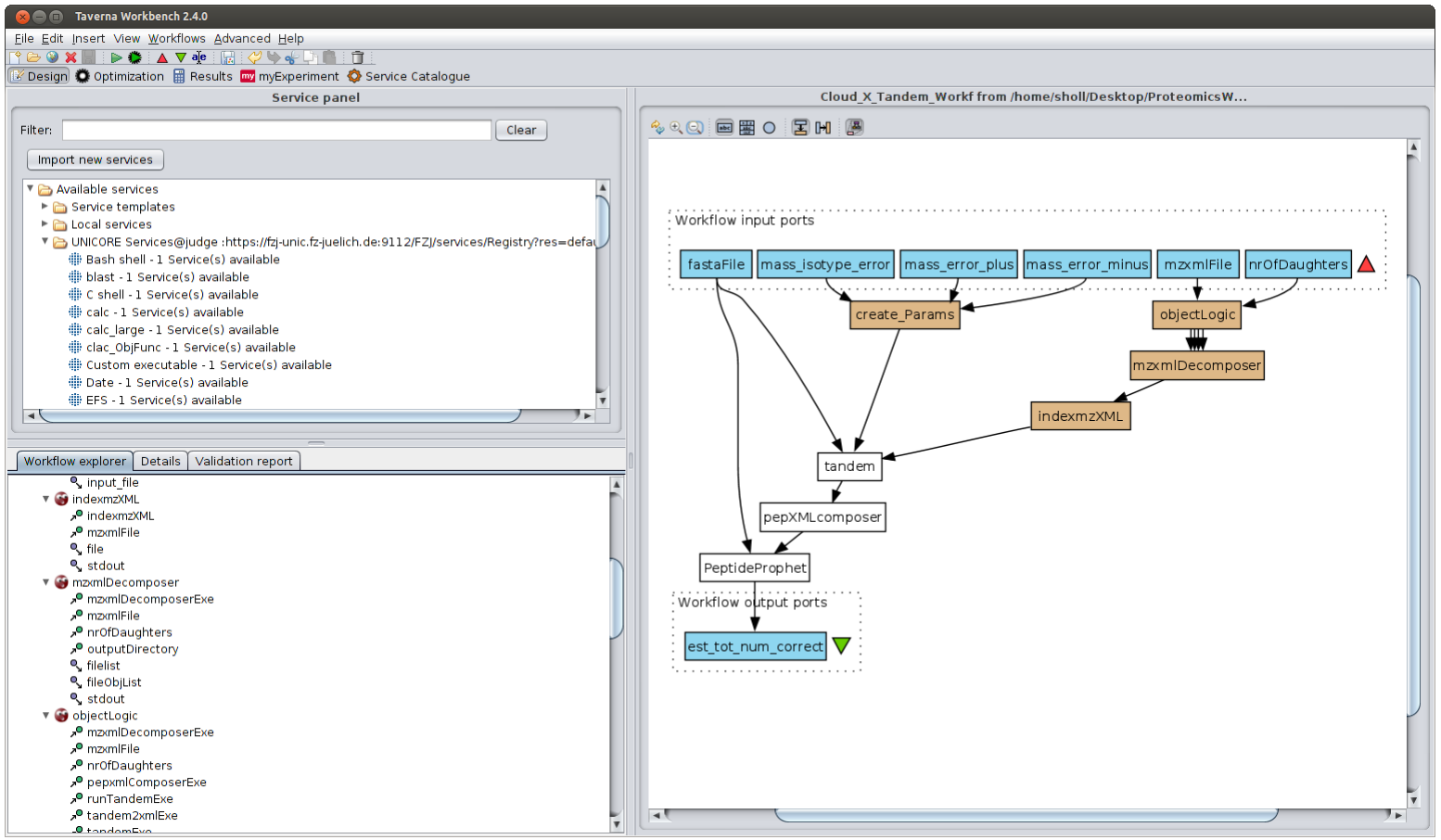
UNICORE Grid Middleware

- Client and Server software
- Seamless and secure access to HPC resources
- Based on open standards: X.509, SAML, XACML, WS-*
- Service Oriented Architecture (SOA) and Web Services Resource Framework (WS-RF) compliant
- Support Grid Standards (JSDL, OGSA-BES)

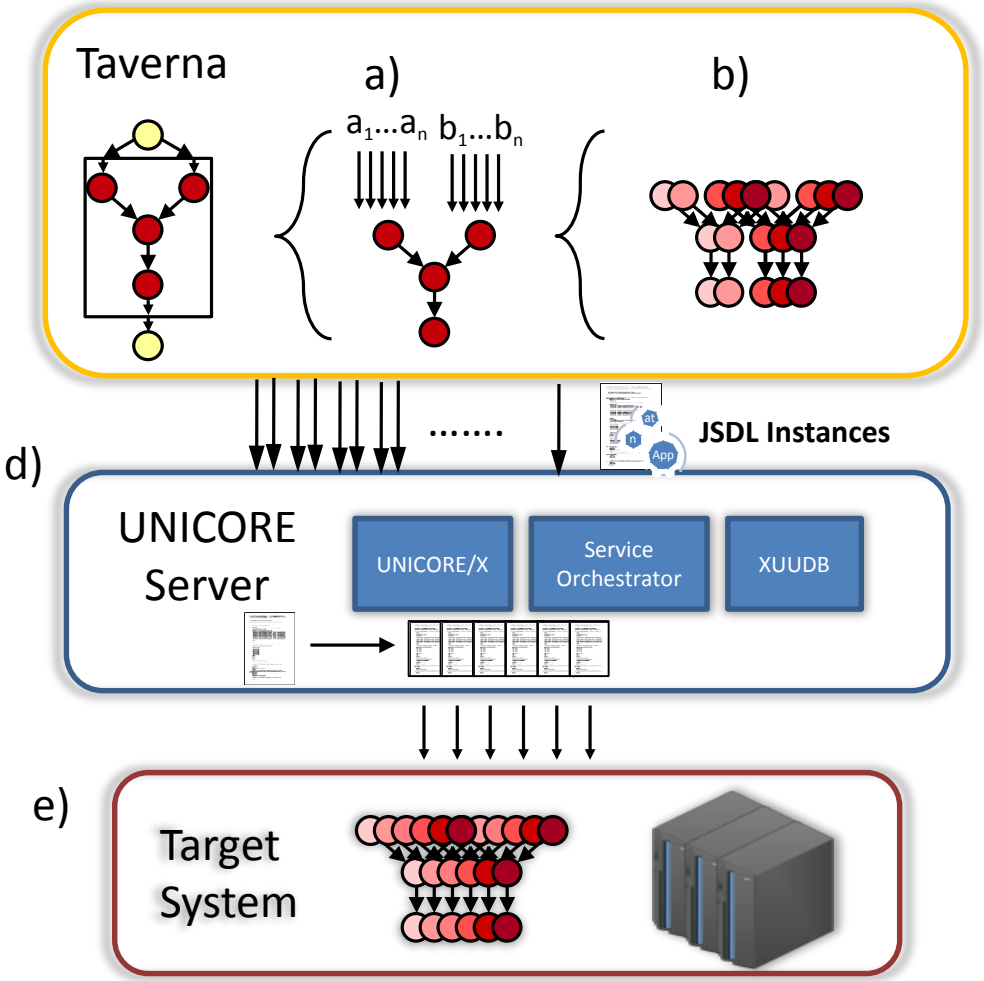


Use Case: Advanced Workflow Optimization

- The choice of parameters has a tremendous impact on overall scientific experimentation – performed via workflows
- Choose the best parameters instead of default ones
  - Default parameters ⇨ Weak scientific results
- Proof of concept: Taverna – UNICORE plugin has been implemented to optimize workflow parameters by applying Genetic Algorithms
- Sub-workflows are considered for the optimization
- Several instances are executed in parallel
  - Each instance with one parameter sample
  - The resultant values are taken as fitness



Job Generation and Submission

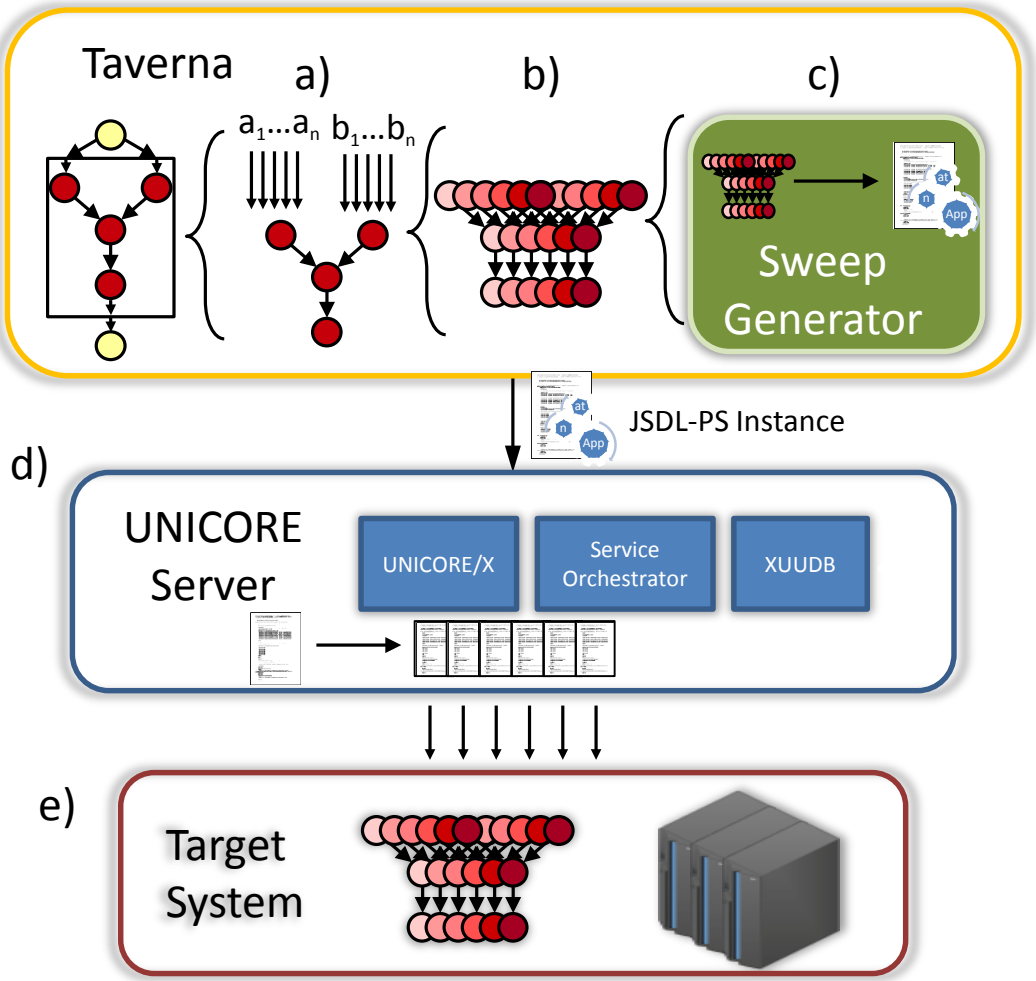


Limitations

- Client manually submits N job (same application) requests, with only difference in application parameters

- Comes with an additional overhead,
  - Client responsible of managing each sweep manually
  - N job status remote call outs
  - Data staging-in for each job
  - Waste of network resources

Parametric Job Generation and Submission



JSDL Parameter Sweep Extensions

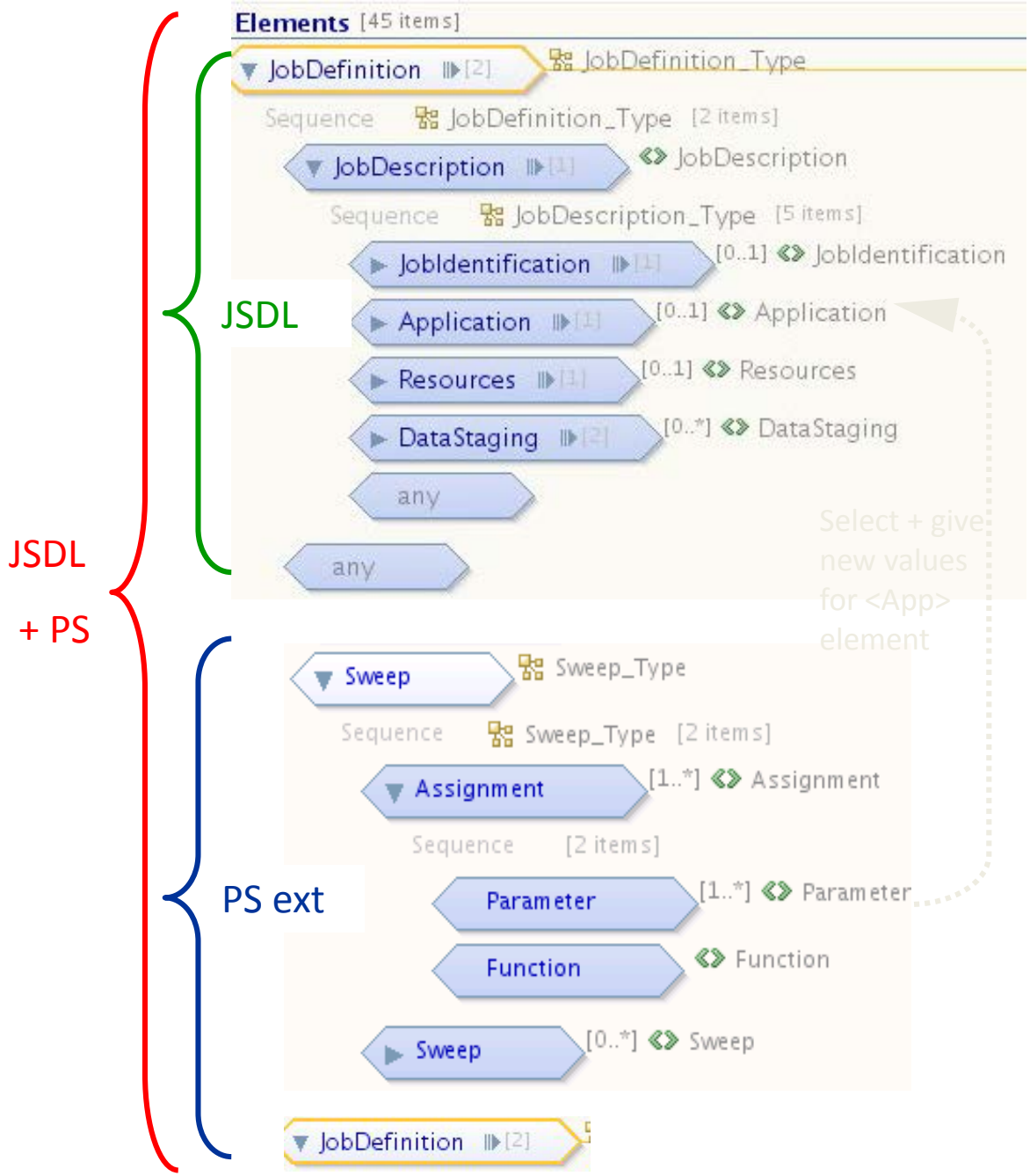
http://forge.gridforum.org/sf/projects/jsdl-wg

1. Extension of Job Submission and Description Language (JSDL) specification [GFD.136]
2. A common requirement to select a job and submit it '10, 50, 300' times, each time making some modifications to the 'original/master' JSDL (e.g. args, parameters, output dir, input file whatever…).
3. The JSDL + PS extensions allows you to group the master JSDL + the required modifications (which JSDL fields require sweeping);
   - Saves writing multiple separate JSDL docs.
   - Can be *any* value within the JSDL document itself,
   - Can be *any* value within a named file that is referenced by the JSDL (e.g. an input file).
   - Actually yields multiple separate jobs (rather than solely parameter sweeps).

Slide Courtesy: Geoff Williams et al.

JSDL Sweep Overview

1. Nest <Sweep> elements within a JSDL doc.
2. The <*Assignment*> identifies which set of <*Parameters*> should be swept / iterated using the given sweep <*Function*>.
3. <Parameter> + <Function> are ***abstract*** (can define different implementations as required).
4. Parameters:
   - DocumentNode
   - FileSweep
5. Functions:
   - Values, LoopInteger, LoopDouble



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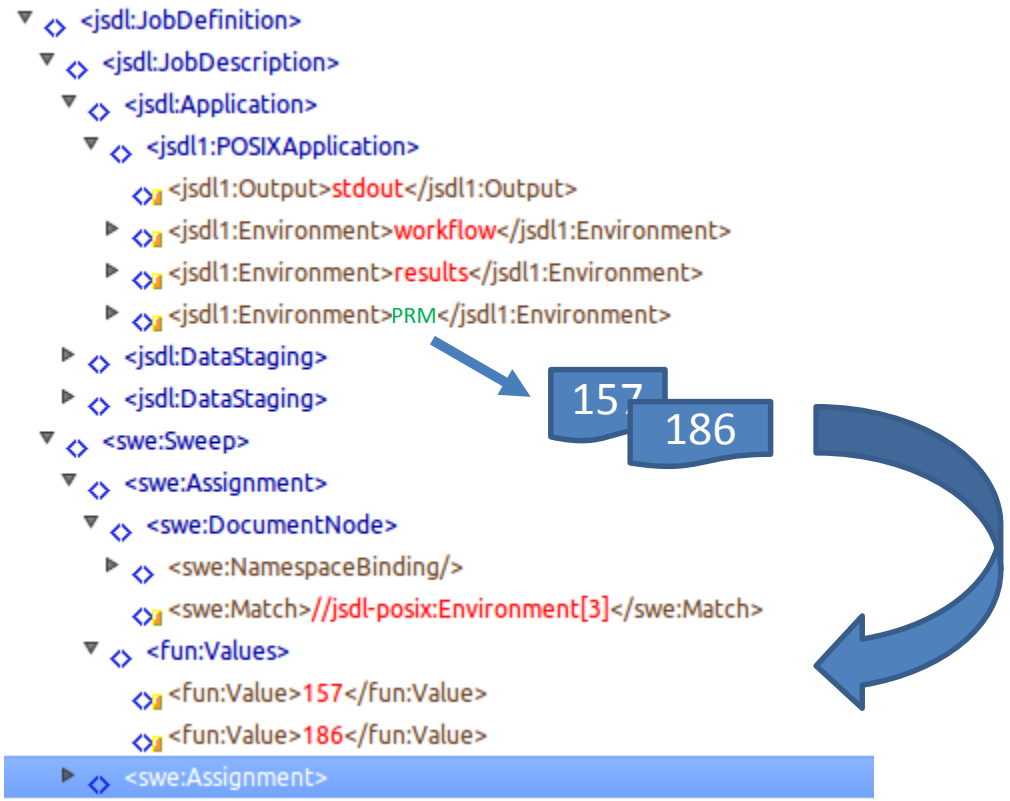
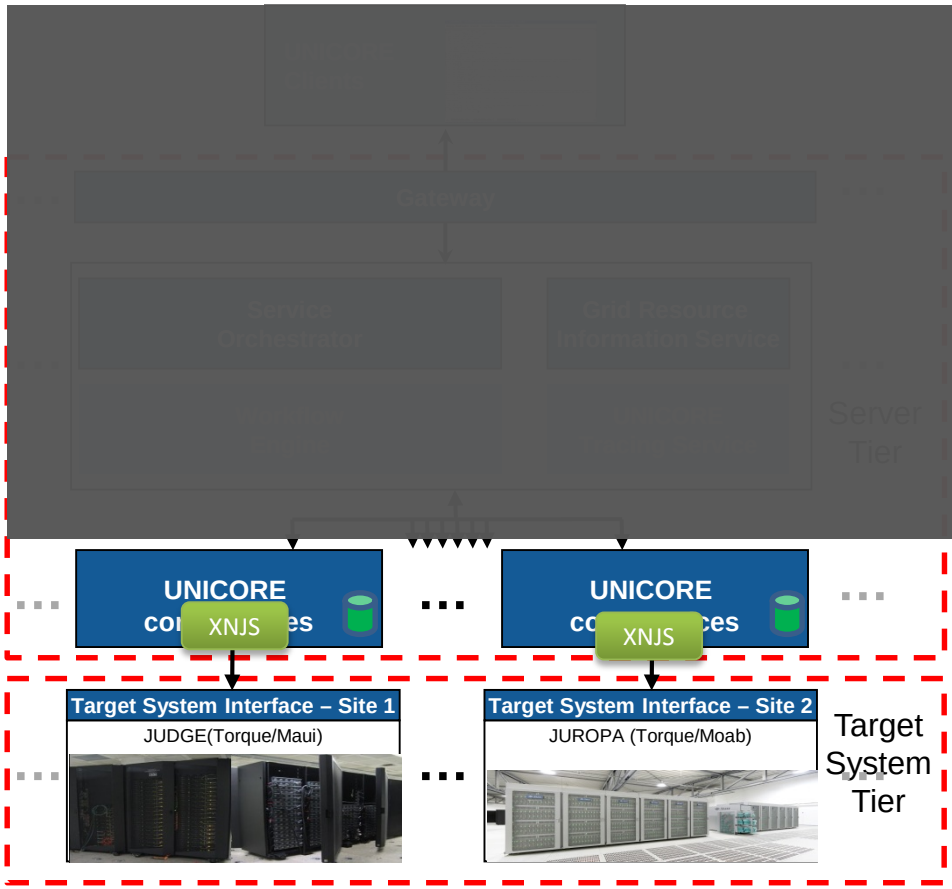
JSDL-PS Example



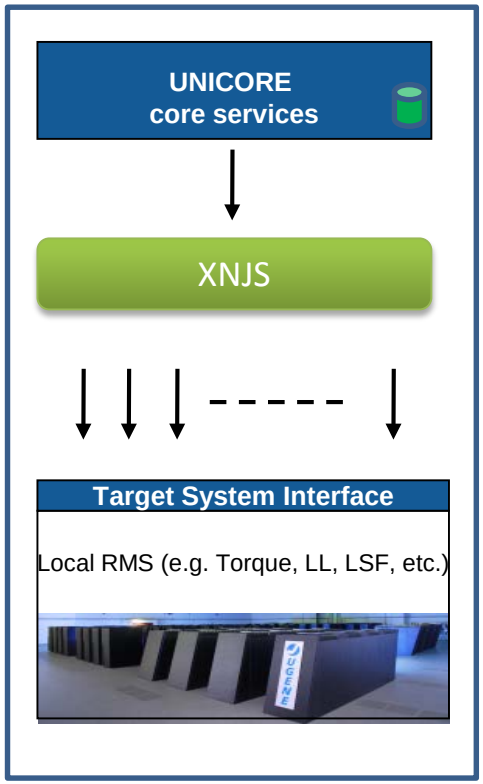
UNICORE Parameter Sweep Implementation

- Job execution service consume JSDL-PS request and pass it to the XNJS
- XNJS parses JSDL and forwards request to the Target System Interface (TSI)
- TSI translates the incoming XNJS message to batch system specific commands

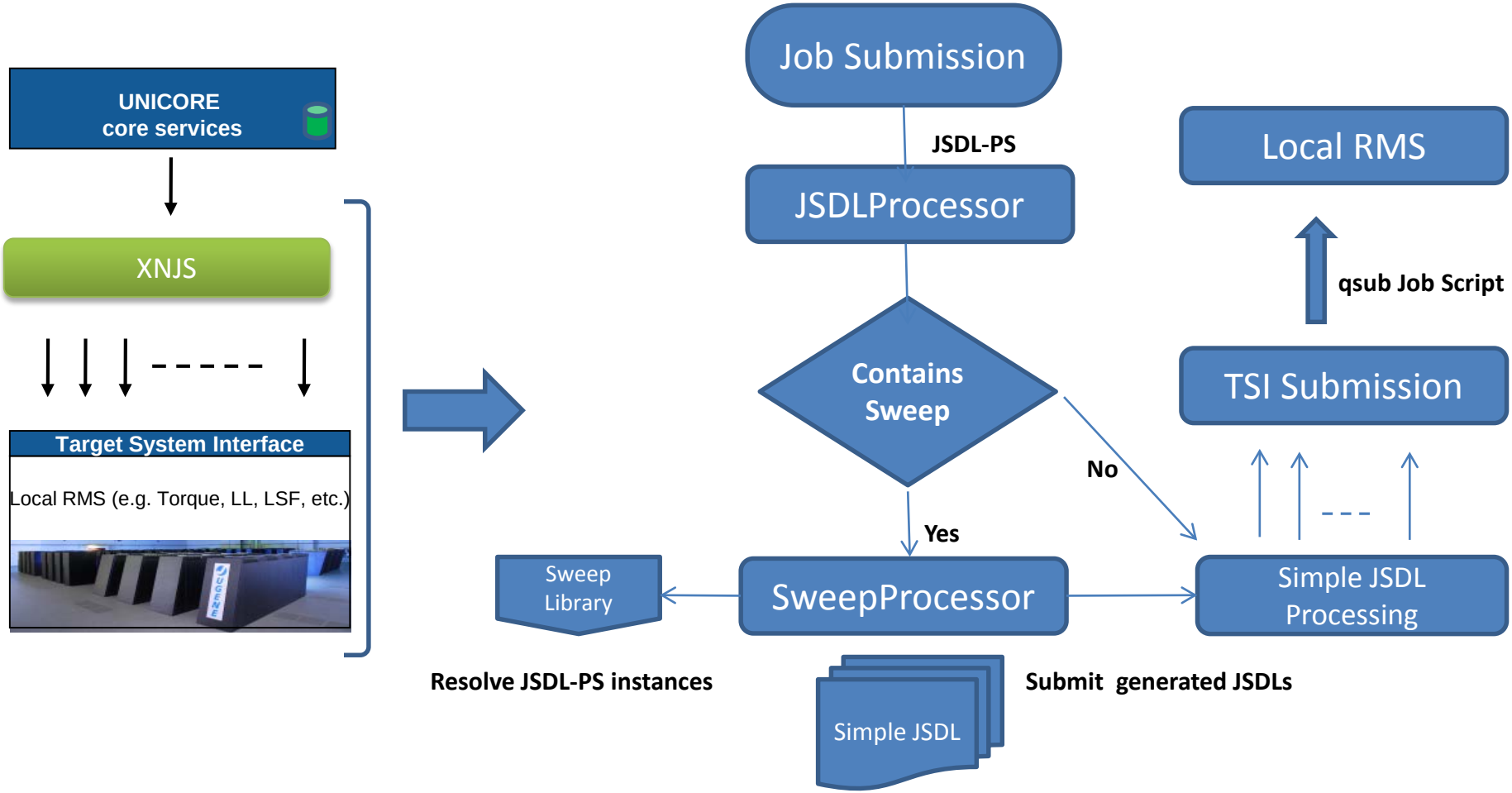


XNJS Execution Management System

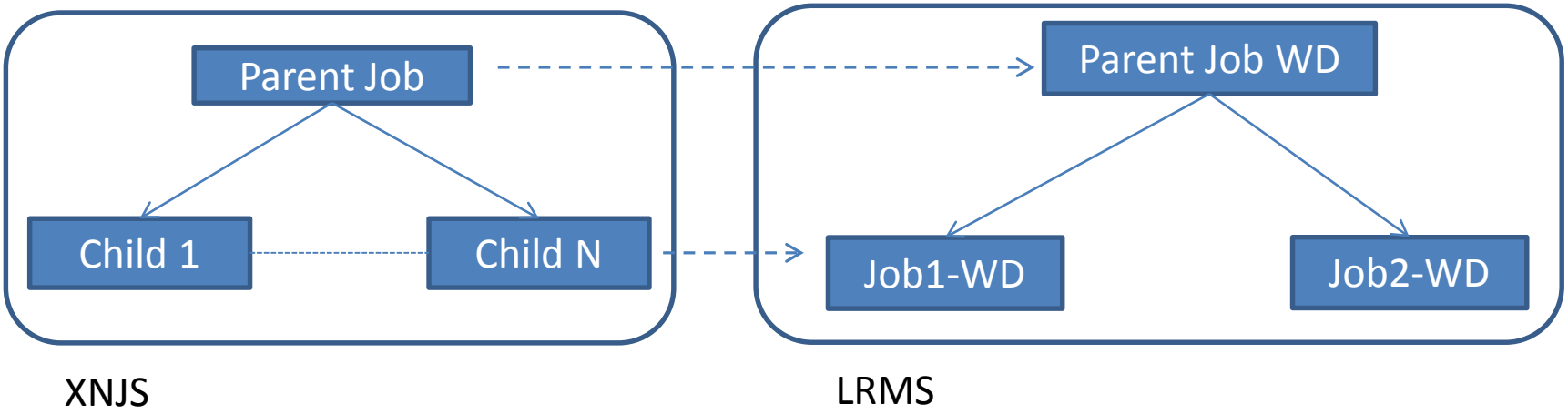
- Separated from core (Web) services tier
- Manage life cycle of atomic jobs (stage-in, execute, stage-out)
- Perform JSDL parsing
- Validation against resource and job requirements
- Manage user access to jobs
  - submit, start, stop
- Support file spaces (Job Working Directory, HOME, ROOT)



XNJS Sweep Job Handling

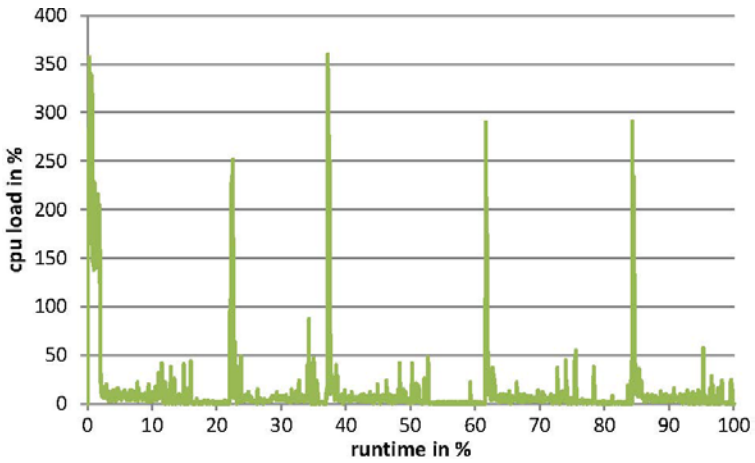


XNJS Job Working Directory Structure

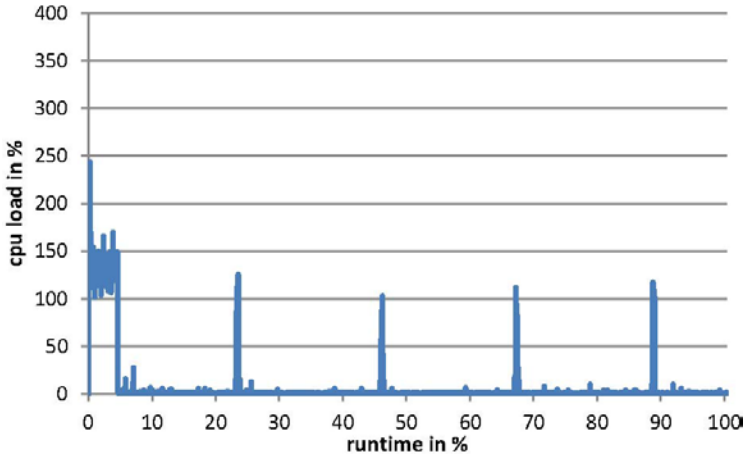


- Parent Job Working Directory is used for file staging-in
  - Files are staged-in once to the parent job WD
- Soft links of the each staged-in file is created in the child job working directories

Client Performance Impact



Conventional Submission



Sweep Submission

Conventional vs Sweep

	File upload (small example)	File upload (large example)	Average CPU load on the client (%)	Max. CPU load on the client (%)
Conventional Submission	400 kB	700 MB	12.89	360
Sweep Generator	20 kB	35 MB	7.79	244

Conclusions

- Parametric job run is optimized by submitting one remote job in lieu of hundreds or thousands
- JSDL-PS implementation will benefit wide range of applications which are relying on workflow optimization
- Taverna UNICORE plugin is extended to use the server side parameter sweep capabilities
- Future Directions
  - More intuitive file staging-ins
  - Combining standard out / err
  - Meaningful job status reports

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Questions?