Serpens suite for Kepler workflow orchestration system

Marcin Plociennik (PSNC)
Michal Owsiak (PSNC)
Tomasz Zok (PSNC)
Outline

(1) Kepler overview
(2) Use cases
(3) Serpens
(4) Summary
Kepler overview

www.kepler-project.org

- Scientific Workflow System
- Builds upon the open-source Ptolemy II framework
- Current release: 2.2 (past 2.1, 1.0 – May 2008), initiated 2003
- Allows scientists to visually design and execute scientific workflows
- Actor-oriented model with directors acting as the main workflow engine
- Enables different models of computation
- Workflows are saved as XML files - can easily be shared/published
- Kepler is supported by the NSF-funded Kepler/CORE team, which spans several of the key institutions that originated the Kepler project: UC Davis, UC Santa Barbara, and UC San Diego
What flows through object is streams of data

Adapted from B. Ludaescher

Input data

<table>
<thead>
<tr>
<th>actor name</th>
</tr>
</thead>
<tbody>
<tr>
<td>data (state)</td>
</tr>
<tr>
<td>parameters</td>
</tr>
<tr>
<td>ports</td>
</tr>
</tbody>
</table>

Output data
Main components

![Diagram showing components and relationships](image-url)
Actors perform actions basing on input ports and parameters

Expression

input + 2

Display

String Constant

Hello World
Kepler workflows are used extensively by fusion physics community. Many use cases were developed in EUFORIA project (EU Fusion fOR Iter Applications) and are supported by EGI-InSPIRE project (SA3).

http://www.euforia-project.eu/

The distributed computing middleware used by EUFORIA: UNICORE and gLite.
**BIT1** is a code that solves the plasma transport in a divertor. BIT1 is a 1D in real space and 3D in velocity space that takes into account the different relevant phenomena that happen in the scrape-off-layer. It is used to study properties of the plasma-wall transition (PWT) change.

Two use cases implemented and used as Kepler workflows:

- Parallel MPI run on HPC resources via UNICORE.
- Concurrent parameter scan on multiple grid nodes.
HELENA-ILSA applications

**HELENA** is a high resolution fixed boundary equilibrium code used to calculate the magnetic flux surfaces in a tokamak. This involves solving a large sparse band matrix equation iteratively.

**ILSA** is used to compute linearly unstable Magnetohydrodynamics (MHD) modes in tokamak plasma.

Two use cases implemented and used as Kepler workflows:
- Single HELENA on grid, multiple ILSA on grid.
- Single HELENA on grid, parallel ILSA on HPC.
HELENA-ILSA applications
Successful implementation of workflows:

- **EUFORIA-DEISA**
  - Execution of real scientific applications on a DEISA HPC facility
- **EUFORIA-EGEE**
  - Execution of real scientific applications on EGEE infrastructure
- **EUFORIA-DEISA-EGEE**
  - Workflow managing job execution in mixed DEISA and EGEE environment
Serpens suite for Kepler

- **Serpens:**
  - Actors, workflows, templates for using grid middleware:
    - gLite
    - Unicore
    - QCG
  - Accessing cloud:
    - OpenNebula
    - Amazon EC2

- Developed under EU FP7 Euforia project
- Used by Fusion community
- Support for new workflow scenarios as a part of EGI-InSPIRE SA3

[http://serpens.psrcn.pl](http://serpens.psrcn.pl)
UNICORE module

Based on UCC. Provides its functionality within Kepler actors.

Contains actors allowing:

- File upload/download,
- Sites/storages listing,
- Job submission (UCC JSON specification or JSDL),
- Status checking,
- Output retrieval.
UNICORE module

Based on UCC. Provides its functionality within Kepler actors.

A full use case workflow:
Job submission → Status checking loop → Output retrieval
Vine Toolkit module

Access to UNICORE via Vine Toolkit server.

Contains actors allowing:

- File upload/download/registration,
- JSDL generation,
- Job submission,
- Status checking,
- Retrieval of standard output/error streams.
Vine Toolkit module

Access to UNICORE via Vine Toolkit server.

A full use case workflow:
Inputs upload → Outputs registering → JSDL generation → Job submission → Status Checking → Output retrieval
Serpens suite

All modules and external libraries are available under BSD license or compatible.

Serpens was successfully validated by Kepler developers and was incorporated within its official repository.

Serpens belongs to Distributed Execution interest group and as such is listed on Kepler webpage.

http://serpens.psnc.pl/
Serpens suite

Current Suite

Available Suites:
- kepler-2.2
- master-slave-2.2
- module-manager-gui-2.2
- provenance-2.1
- reporting-2.1
- serpens-2.2
- tagging-2.1
- workflow-run-manager-2.1

Selected Modules:

Available Modules:
- ssh-2.0.0
- ssh-2.1.0
- tagging-2.1.0
- uniscore-2.2.0
- util-2.0.0
- util-2.1.0
- vine-toolkit-2.2.0
- workflow-run-manager-2.1.0

Show suite patches.

Show test releases.

Automatically check for patches on startup.

Check for Patches Now

Rollback Kepler

Apply and Restart
Thank you for attention!

Participants interested in using Serpens are welcome to check our official webpage or contact us directly.

http://serpens.psnc.pl
marcinp@man.poznan.pl