AEGIS CMPC
Scientific Gateway

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Overview

- AEGIS CMPC Applications
- AEGIS CMPC Architecture
- gUSE/WS-PGRADE Portal
- AEGIS CMPC Scientific Gateway
- AEGIS CMPC Database Backend
- AEGIS CMPC DCI
- Acknowledgment
- References
AEGIS CMPC Applications

- **AEGIS**
  Academic and Educational Grid Initiative of Serbia
- **CMPC**
  Condensed Matter Physics Community
- **AEGIS CMPC SG**
  Provides access to three applications
  - **SPEEDUP**
    Monte Carlo (MC) based path integral algorithm for calculation of quantum mechanical transition amplitudes for 1D models.
  - **QSPEEDUP**
    quasi-Monte Carlo (MC) based path integral algorithm for calculation of quantum mechanical transition amplitudes for 1D models.
  - **GP-SCL**
    Set of codes for calculating both stationary and non-stationary solutions of the time-dependent Gross-Pitaevskii (GP) equation in one, two, and three space dimensions in a trap using imaginary-time and real-time propagation.
AEGIS CMPC ARCHITECTURE [1/2]

Architecture consists of four main components:

- AEGIS CMPC gUSE/WS-PGRADE Portal
- AEGIS CMPC Database backend
- AEGIS CMPC Scientific Gateway
- CMPC.AEGIS.RS DCI (EMI/gLite based)

AEGIS CMPC Scientific Gateway
- End user interface
- Google Web Toolkit

AEGIS CMPC gUSE/WS-PGRADE Portal
- Workflow Interpreter
- DCI Bridge
- Remote API
- Localhost resource
- Distributed Computing Resources
  - gLite middleware (cmpc.aegis.rs)

CouchDB

RESTful web service

Job submission engine

AEGIS CMPC DB
AEGIS CMPC Architecture [2/2]

- Architecture provides two main interfaces
  - End user interface
  - Workflow developer interface

End user interface:
- Google Web Toolkit

Workflow developer interface:
- Workflow submission
- Workflow output

AEGIS CMPC Scientific Gateway
- End user interface

AEGIS CMPC gUSE/WS-PGRADE Portal
- DCI Bridge
  - localhost resource

AEGIS CMPC DB
- CouchDB

Job submission engine
- DCI Bridge
  - gLite middleware (cmpc.aegis.rs)

RESTful web service
- workflow submission
- workflow output

New configuration
**Workflow Developer Interface**


(Q)SPEEDUP Workflow:

- **Preparation**
  
  DB > JSON conf. > APP. conf. + APP. stream mng.

- **Execution**
  
  APP. job submission to EMI/gLite-based infrastructure

- **Result Publication**
  
  APP. output + TECH. metadata > JSON output > DB
End user interface provides

- Summary of collected numerical results per configuration of the physical system
- Querying of available physical system configuration
- Submission of new physical system configuration
- Allows overview of the results without authentication
- Performs authentication for the submission of new configuration

Developed in Google Web Toolkit environment

Deployed through the Apache Tomcat engine
AEGIS CMPC Database Backend

- **Document-oriented database**
  - CouchDB technology
- **CouchDB RESTful web-service**
- **extended with three layers**
  - AuthN/AuthZ layer
  - Tracking layer
  - Merging layer
- **AuthN/AuthZ**
  - username/password
  - X.509 cert.
  - X.509 proxy cert.
- **Predefined JSON structures**
  - speedup_cfg
  - speedup_job
  - speedup_out
  - QSpeedup_cfg
  - etc.
- **Dedicated VO:** cmpc.aegis.rs
  
  https://voms.ipb.ac.rs:8443/voms/cmpc.aegis.rs

- **CMPC.AEGIS.RS** supported by
  - 6 production sites
  - More than 1000 CPUs
  - More than 30 TBs

- **Application binaries**
  preinstalled in VO software
  area on each Grid site
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