

AEGIS CMPC SCIENTIFIC GATEWAY

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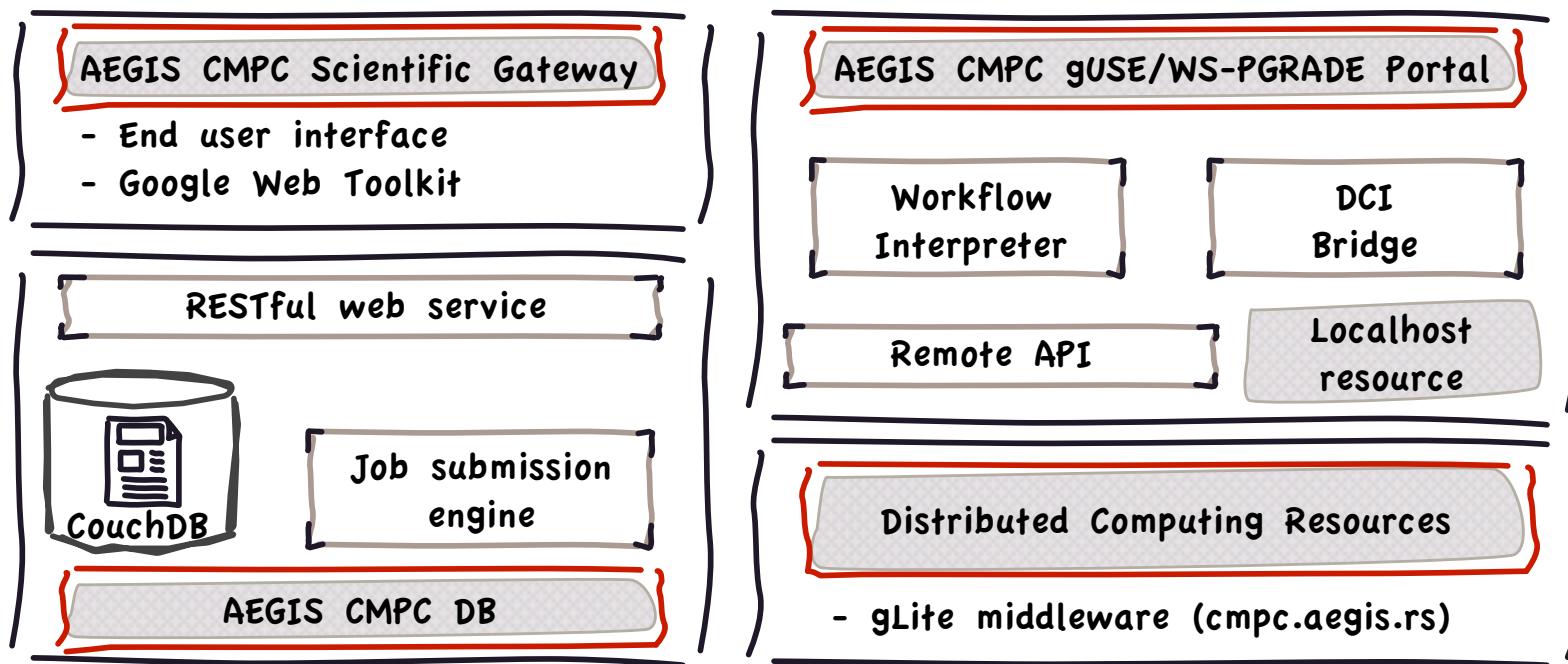


- AEGIS CMPC APPLICATIONS
- AEGIS CMPC ARCHITECTURE
- GUSE/WS-PGRADE PORTAL
- AEGIS CMPC SCIENTIFIC GATEWAY
- AEGIS CMPC DATABASE BACKEND
- AEGIS CMPC DCI
- ACKNOWLEDGMENT
- REFERENCES

- **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.

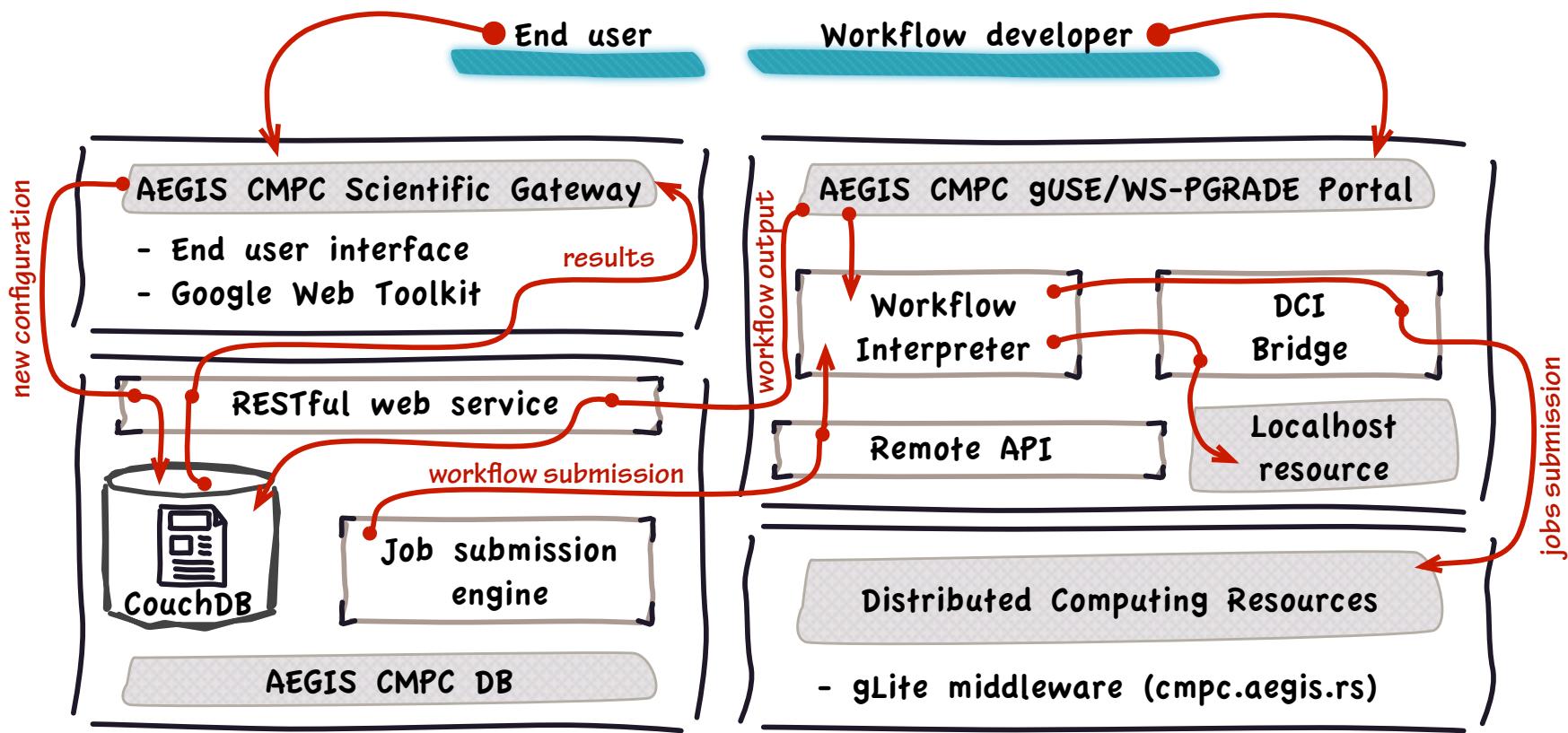
AEGIS CMPC ARCHITECTURE [1/2]

- 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 ARCHITECTURE [2/2]

- ARCHITECTURE PROVIDES TWO MAIN INTERFACES
 - END USER INTERFACE
 - WORKFLOW DEVELOPER INTERFACE



AEGIS CMPC GUSE/WS-PGRADE PORTAL

■ WORKFLOW DEVELOPER INTERFACE

[HTTP://SCI-BUS.IPB.AC.RS:8080/LIFERAY-PORTAL-6.1.0/](http://sci-bus.ipb.ac.rs:8080/liferay-portal-6.1.0/)

■ (Q)SPEEDUP WORKFLOW:

■ PREPARATION

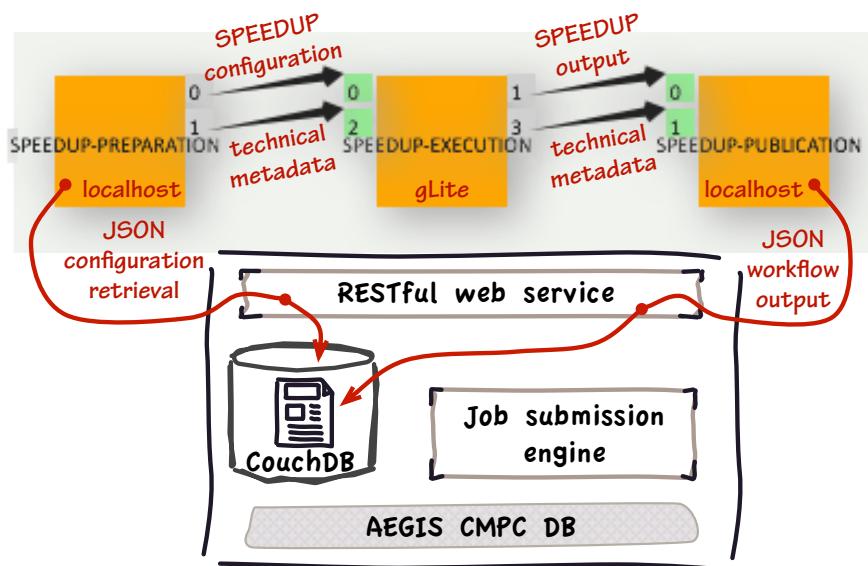
DB > JSON CONF. > APP. CONF. + APP. STREAM MNG.

■ EXECUTION

APP. JOB SUBMISSION TO EMI/GLITE-BASED INFRASTRUCTURE

■ RESULT PUBLICATION

APP. OUTPUT + TECH. METADATA > JSON OUTPUT > DB

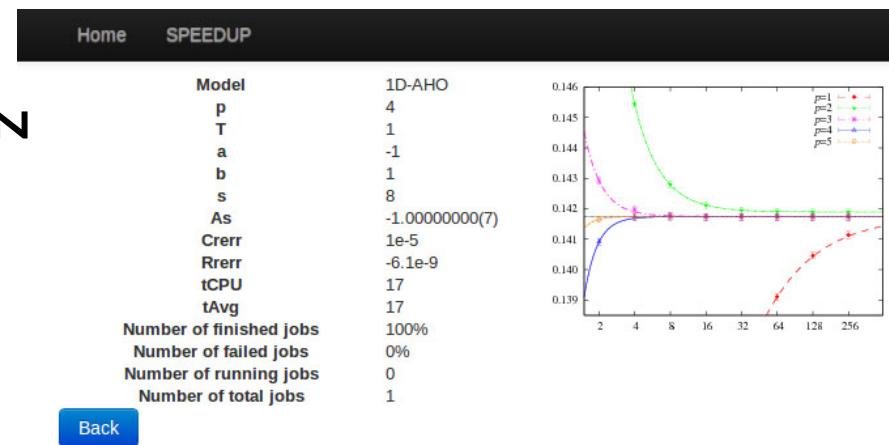


Screenshot of the Liferay Portal interface showing the SPEEDUP workflow instance. The top navigation bar includes 'Welcome', 'Workflow', 'Storage', 'Settings', 'End User', 'Information', 'Statistics', 'Publications', 'Help', and 'Security'. The current page is 'Workflow > Concrete'. The workflow details pane shows the following information:

Workflow name:	SPEEDUP		
Note:	2013-4-22		
Workflow Graph:	SPEEDUP		
Workflow status:	2013-4-22 1:8 Finished		
Selected WF Instance:	2013-4-22 1:8		
Job	Status	Instances	Actions
SPEEDUP-PREPARATION	Finished	1	View finished Hide
SPEEDUP-EXECUTION	Finished	1	View finished Hide
SPEEDUP-PUBLICATION	Finished	1	View finished Hide

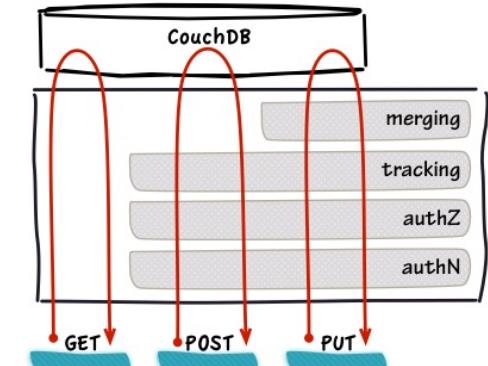
Below the workflow details, there are three tables, each corresponding to one of the workflow steps (SPEEDUP-PREPARATION, SPEEDUP-EXECUTION, SPEEDUP-PUBLICATION). Each table lists resources and their status (e.g., finished, error), along with links for 'View info', 'Logbook', 'std. Output', 'std. Error', and 'Download file output'.

- **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.



The screenshot displays the Apache CouchDB Futon interface. On the left, there's a sidebar with a red 'X' logo and the text 'CouchDB relax'. The main area shows a table with a single row of data. The columns are 'Field' and 'Value'. The 'Field' column contains '_id', '_rev', 'document_publisher', 'error', 'reason', and 'views'. The 'Value' column contains the document's content, which includes fields like '_id', '_rev', 'address', 'author', 'utc_datetime', 'utc_timestamp', and a 'cfg' section with a map function. A 'Fields' tab is selected at the top right of the table.

```
{  
    total_rows: 1,  
    offset: 0,  
    rows: [  
        {  
            id: "d93db3439ea79efd8cc423e84100078f",  
            key: 1366587350,  
            value: {  
                _id: "d93db3439ea79efd8cc423e84100078f",  
                _rev: "1-b9c067ddc6a57df33ec0f46e2dcd9ce",  
                error: "not_found",  
                reason: "missing",  
                type: "speedup_cfg",  
                speedup_cfg: {  
                    model: "LD-AHO",  
                    p: "5",  
                    T: "10",  
                    a: "0.0",  
                    b: "1.0",  
                    s: "5",  
                    Nmc: "1000000",  
                    seed: "123",  
                    stream: "1",  
                    par: [  
                        "1.0",  
                        "2.0"  
                    ]  
                },  
                document_publisher: {  
                    address: "178.148.231.69",  
                    author: "/C=RS/0=AEGIS/OU=Institute of Physics Belgrade/CN=Dusan Vudragovic/CN=800090291",  
                    utc_datetime: "Sun Apr 21 23:35:35 2013",  
                    utc_timestamp: 1366587333  
                }  
            }  
        }  
    ]  
}
```

- DEDICATED VO: CMPC.AEGIS.RS

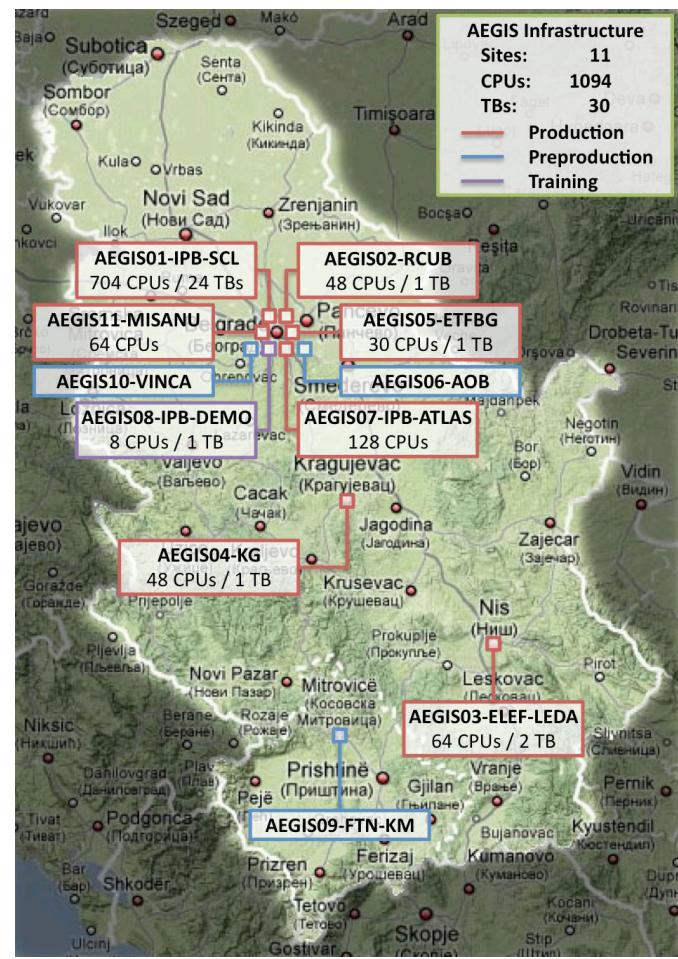
[HTTPS://VOMS.IPB.AC.RS:8443/VOMS/CMPC.AEGIS.RS](https://voms.ipb.ac.rs:8443/voms/cmpc.aegis.rs)

- 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



ACKNOWLEDGEMENT AND REFERENCES

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- D. VUDRAGOVIĆ, I. VIDANOVIĆ, A. BALAŽ, P. MURUGANANDAM AND S. ADHIKARI: "C PROGRAMS FOR SOLVING THE TIME-DEPENDENT GROSS-PITAEVSKII EQUATION IN A FULLY ANISOTROPIC TRAP", *COMPUT. PHYS. COMMUN.* 183 (2012) 2021
- A. BALAŽ, I. VIDANOVIĆ, D. STOJILJKOVIĆ, D. VUDRAGOVIĆ, A. BELIĆ AND A. BOGOJEVIĆ: "SPEEDUP CODE FOR CALCULATION OF TRANSITION AMPLITUDES VIA THE EFFECTIVE ACTION APPROACH", *COMMUN. COMPUT. PHYS.* 11 (2012) 739
- A. BALAŽ, A. BOGOJEVIĆ, I. VIDANOVIĆ AND A. PELSTER: "RECURSIVE SCHROEDINGER EQUATION APPROACH TO FASTER CONVERGING PATH INTEGRALS", *PHYS. REV. E* 79 (2009) 036701
- D. VUDRAGOVIĆ, A. BALAŽ, A. BELIĆ AND A. BOGOJEVIĆ: "QSPEEDUP: QUASI-MC IMPLEMENTATION OF THE SPEEDUP PATH INTEGRAL CODE", PROCEEDINGS OF THE INFOTEH 2010, 17-19 MARCH 2010, P. 73, A-15, JAHORINA, BOSNIA AND HERZEGOVINA
- D. VUDRAGOVIĆ, A. BALAŽ, V. SLAVNIĆ AND A. BELIĆ: "SERBIAN PARTICIPATION IN GRID COMPUTING PROJECTS", PROCEEDINGS OF THE NEC2009, 7-14 SEPTEMBER 2009, P. 286-293, VARNA, BULGARIA