AEGIS CMPC Scientific Gateway

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Overview

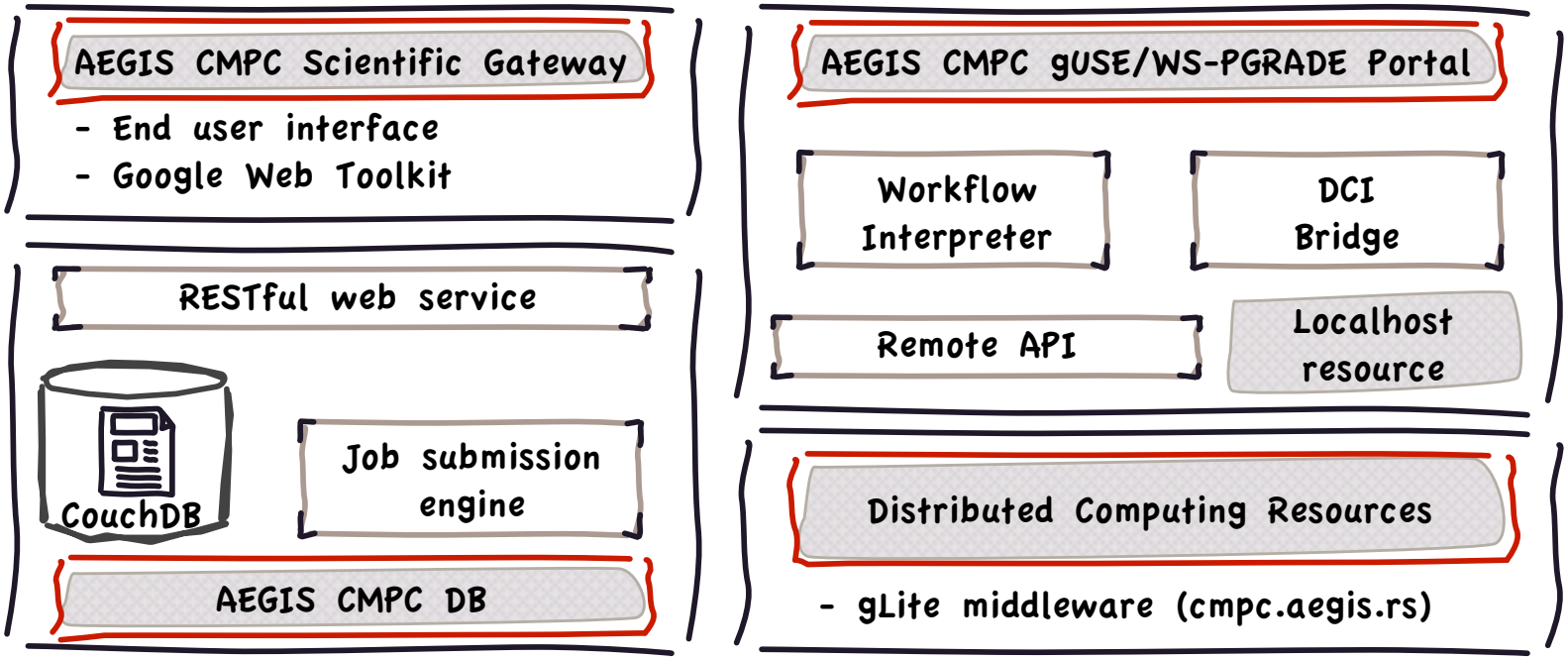
- AEGIS CMPC Applications
- AEGIS CMPC Architecture
- gUSE/WS-PGRADE Portal
- AEGIS CMPC Scientific Gateway
- AEGIS CMPC Database Backend
- AEGIS CMPC DCI
- Acknowledgment
- References

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.

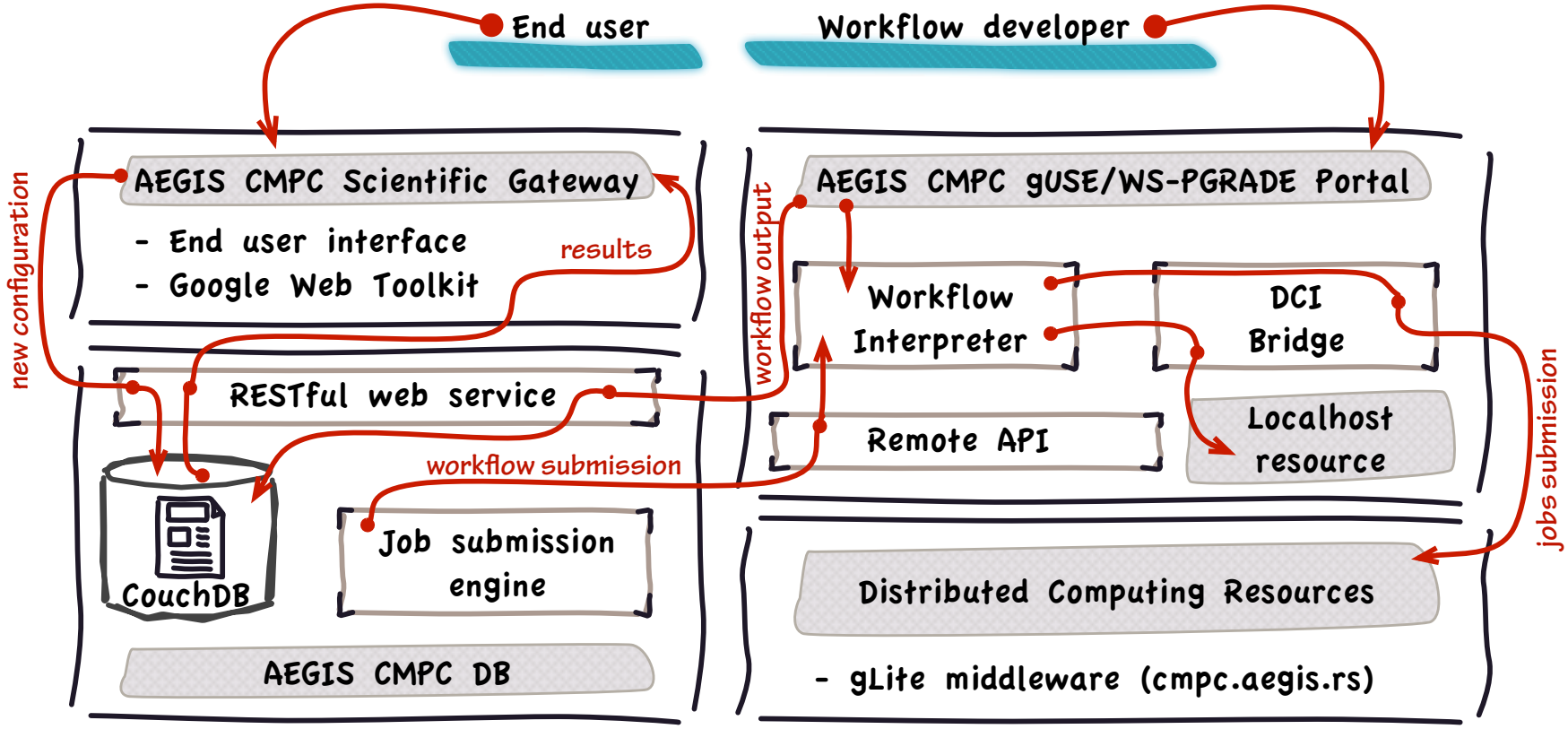
AEGIS CMPC Architecture [1/2]

- Architecture consists of <u>four main components</u>
  - AEGIS CMPC <u>gUSE/WS-PGRADE Portal</u>
  - AEGIS CMPC <u>Database backend</u>
  - AEGIS CMPC <u>Scientific Gateway</u>
  - <u>CMPC.AEGIS.RS DCI</u> (EMI/gLite based)



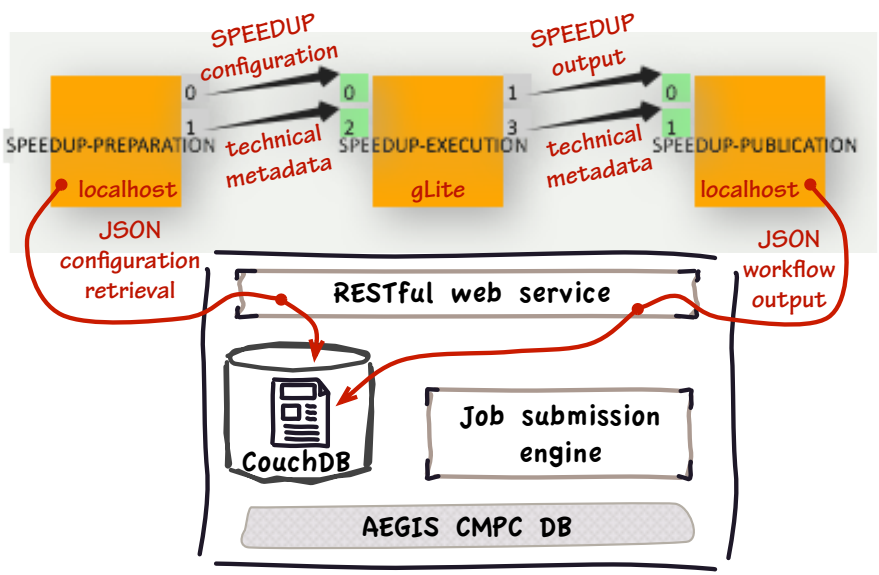
AEGIS CMPC Architecture [2/2]

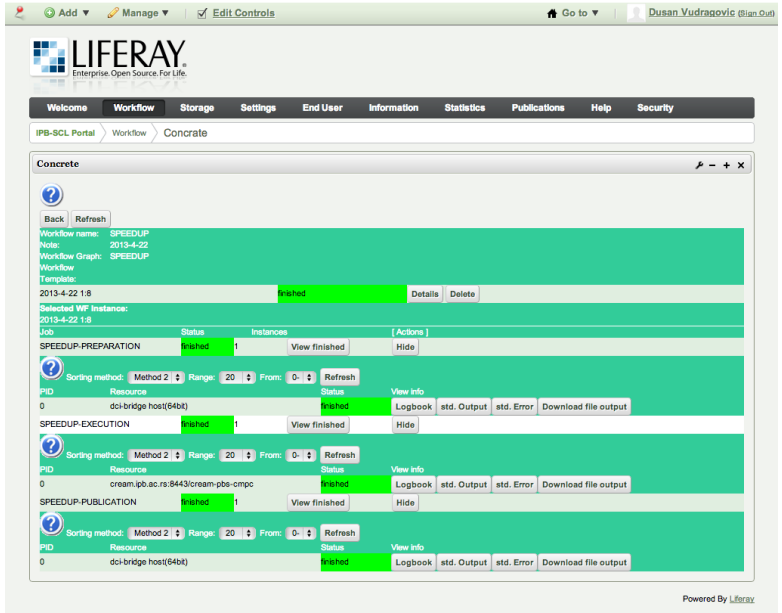
- Architecture provides <u>two main interfaces</u>
  - End user interface
  - Workflow developer interface



AEGIS CMPC gUSE/WS-PGRADE Portal

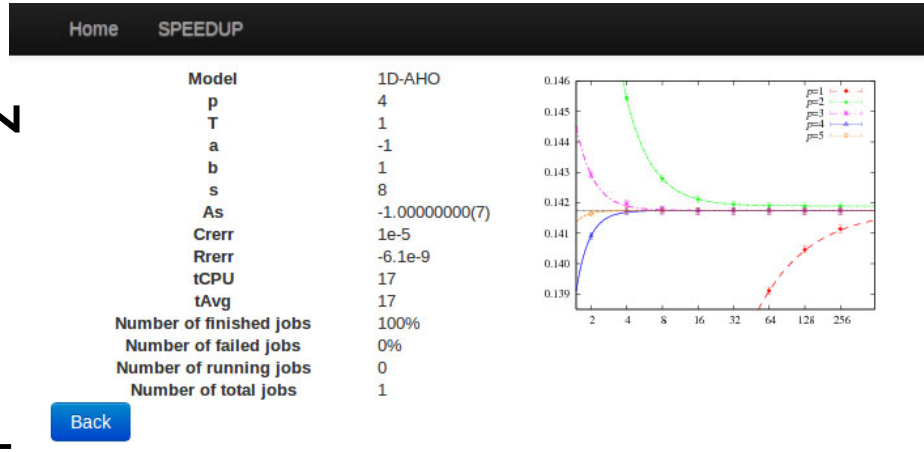
- **Workflow developer interface**
  http://sci-bus.ipb.ac.rs:8080/liferay-portal-6.1.0/
- **(Q)SPEEDUP workflow:**
  - **Preparation**
    DB > JSON conf. > app. conf. + app. stream mng.
  - **Execution**
    App. job submission to EMI/gLite-based infrastructure
  - **Result publication**
    App. output + tech. metadata > JSON output > DB





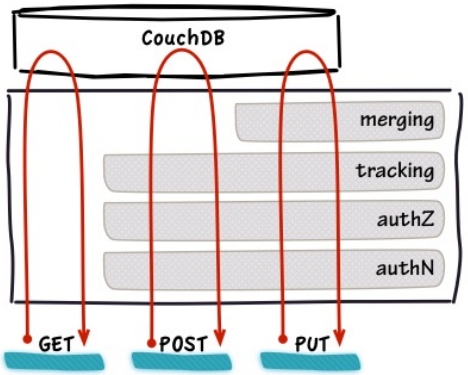
AEGIS CMPC Scientific Gateway

- 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 <u>CouchDB technology</u>
- CouchDB RESTful web-service extended with three layers
  - <u>AuthN&authZ</u> layer
  - <u>Tracking</u> layer
  - <u>Merging</u> layer
- AuthN&AuthZ
  - username/password
  - X.509 cert.
  - X.509 proxy cert.
- Predefined JSON structures
  - speedup_cfg
  - speedup_job
  - speedup_out
  - Qspeedup_cfg
  - etc.

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           reason: "missing",
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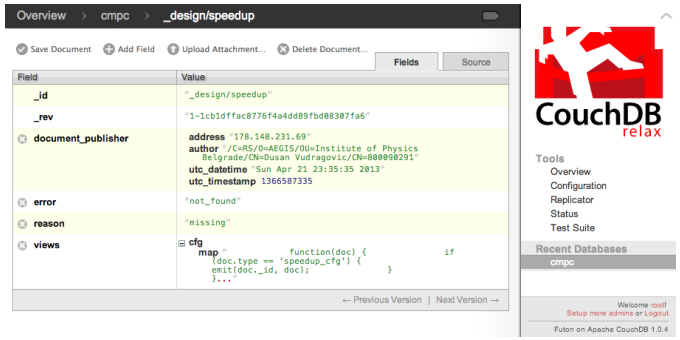
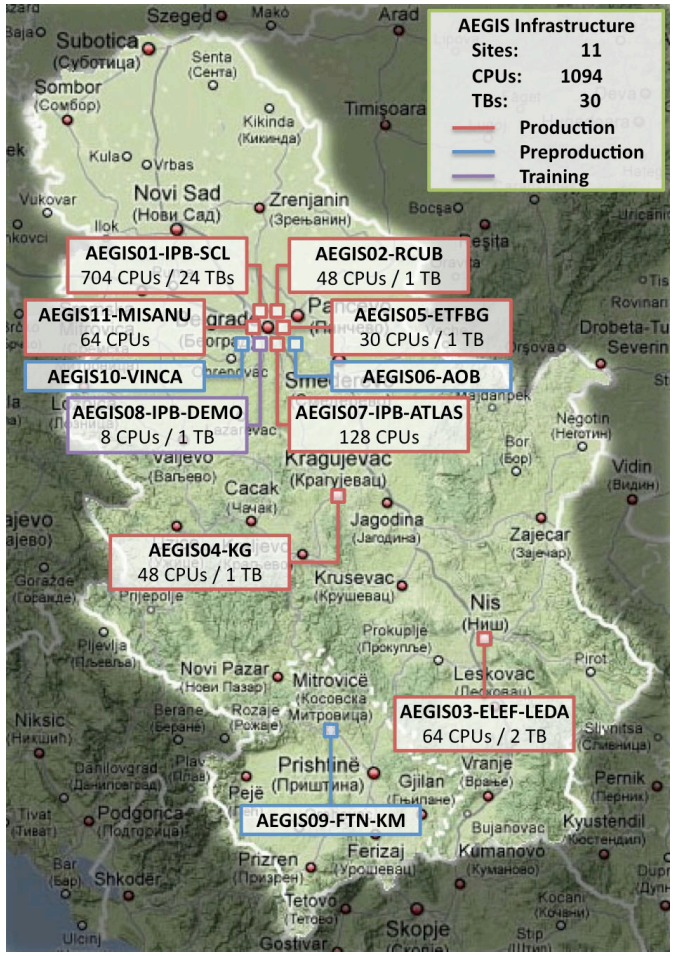


AEGIS CMPC DCI

- 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



Acknowledgement and references

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