

User-friendly access to computational services with FARO portal for EGEE and ENEA-GRID

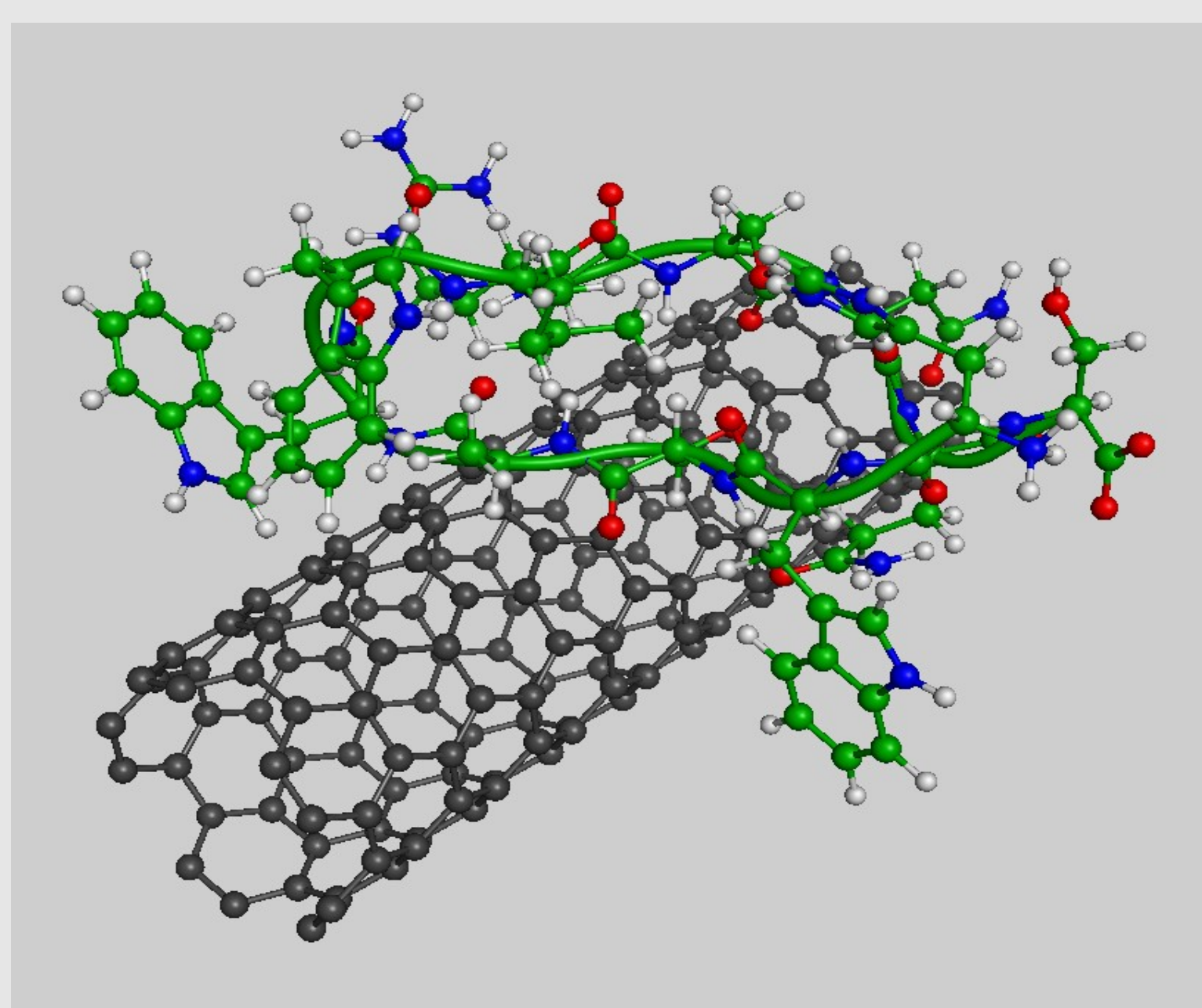
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CPMD

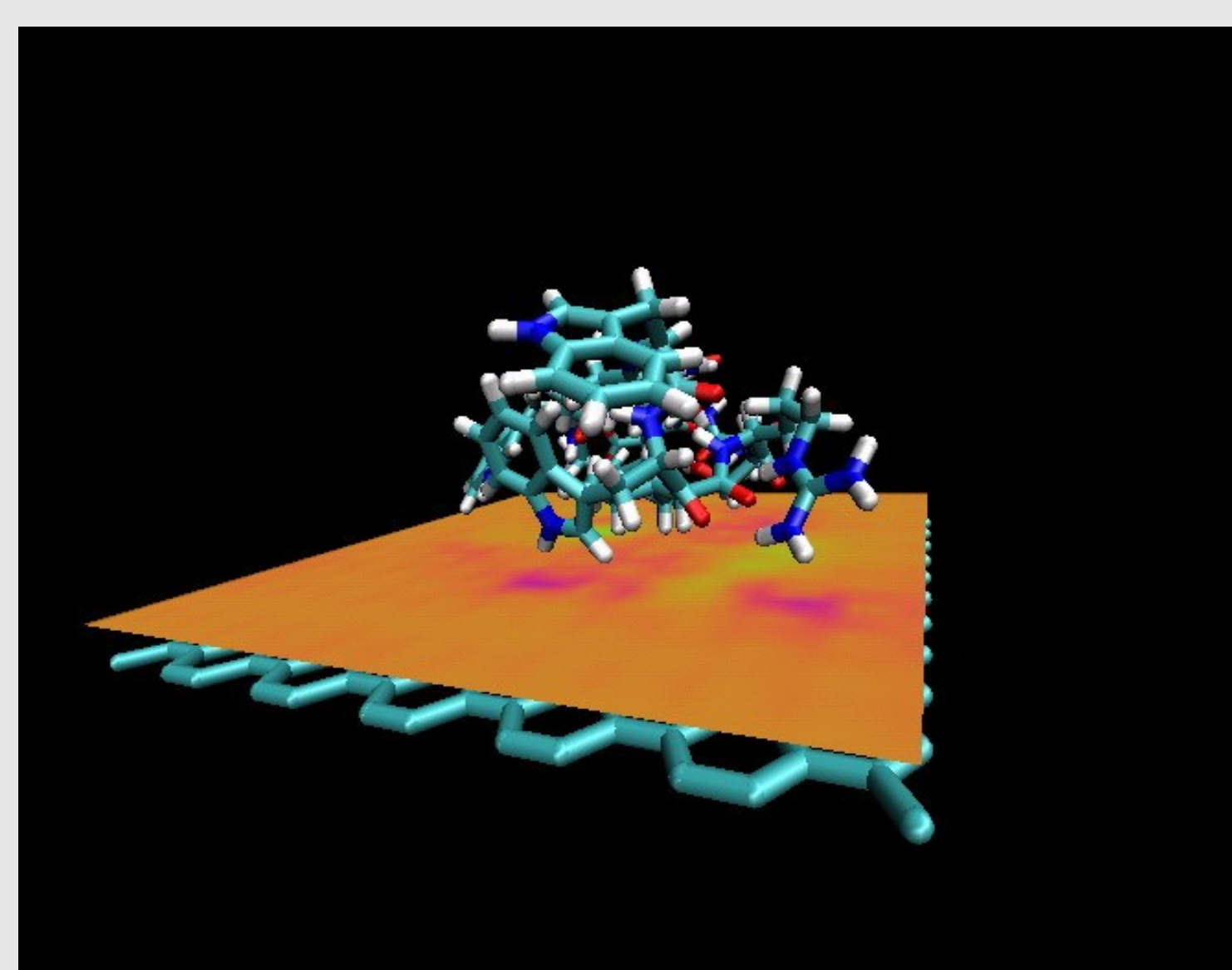
- Parallelized plane wave/pseudopotential implementation of Density Functional Theory
- particularly designed for ab-initio molecular dynamics.

CPMD Job examples



Structural and electronic characterization: graphene and nanotubes

Peptide adhesion on carbon surfaces

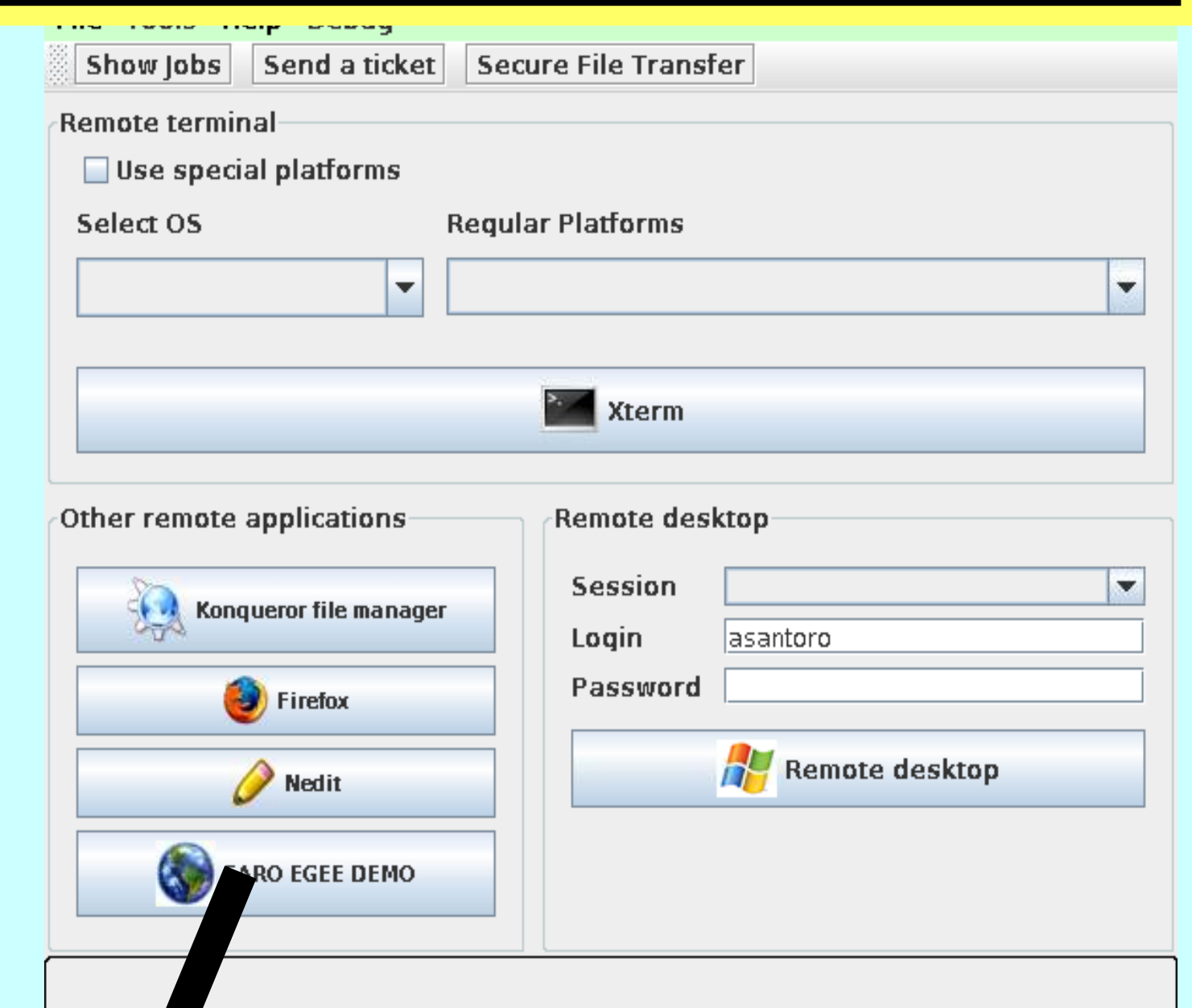


Interface Architecture

- Graphic front-end tailored on the application (CPMD)
- Operational back-end general purpose

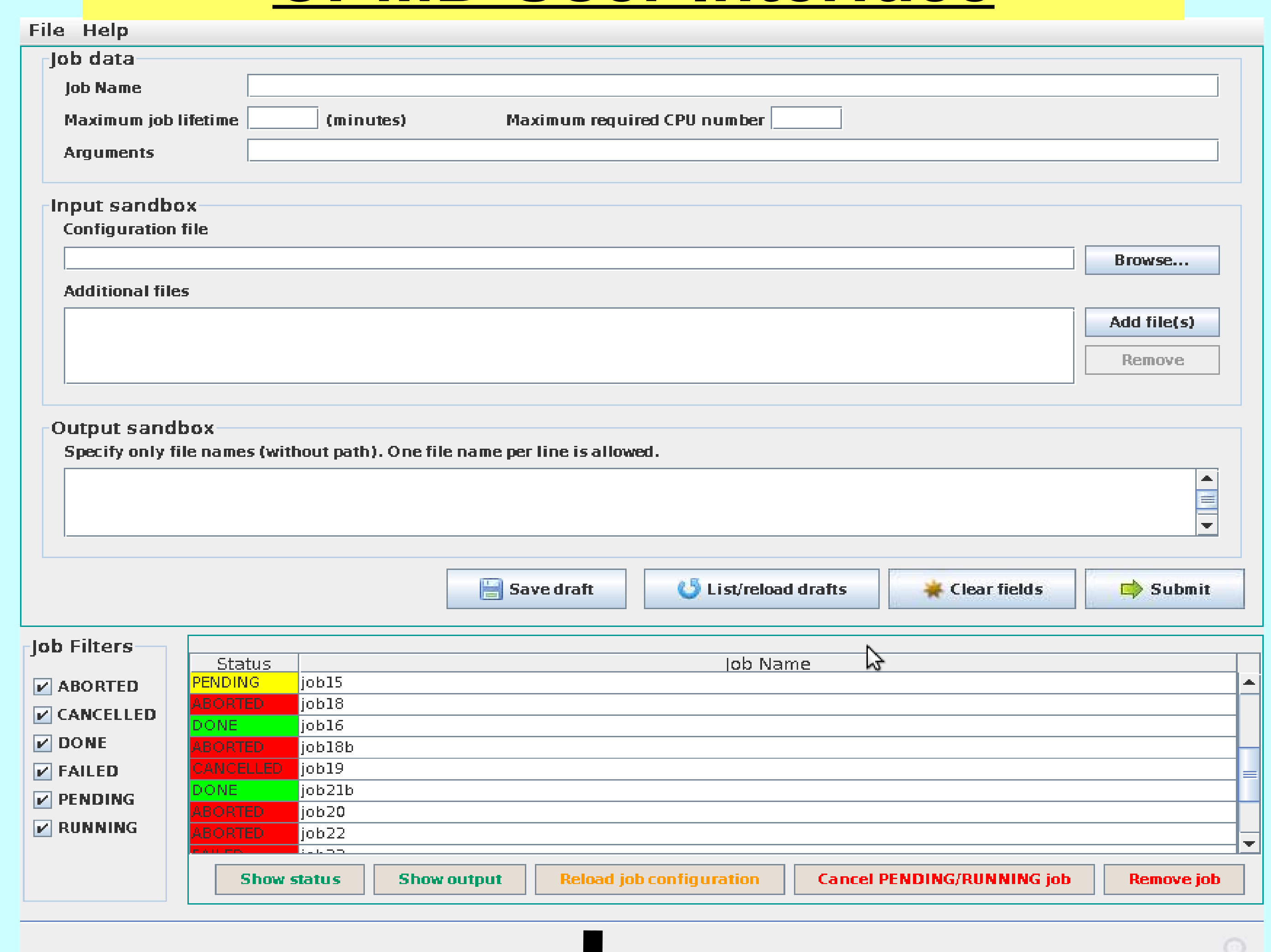
Only the frontend must be modified to create an interface to another application

FARO User Interface



Objective
 CPMD on GRID easily accessible

CPMD User Interface



1. Automatic JDL generation
2. Automatic Job submission
3. Automatic Job state monitoring
4. Automatic output retrieval

JDL generation

- Generated into a specific directory
- Comments on the command line to be used to resubmit the same job

Can be used as a gLite training tool