QCyCAR
Grupo de Química Computacional y Computación de Alto Rendimiento
Universidad de Castilla - La Mancha

CESGA

A General Approach to the Analysis and Design of Grid Portals for Scientific Virtual Organizations

S. Díaz, C. Muñoz-Caro, A. Niño, S. Reyes
QCyCAR. Escuela Superior de Informática
Universidad de Castilla-La Mancha
Ciudad Real. Spain

Outline

- Introduction
- System Requirements analysis
- SVO Grid Portal Architecture
- Experiences
- Aknowledgements

Introduction

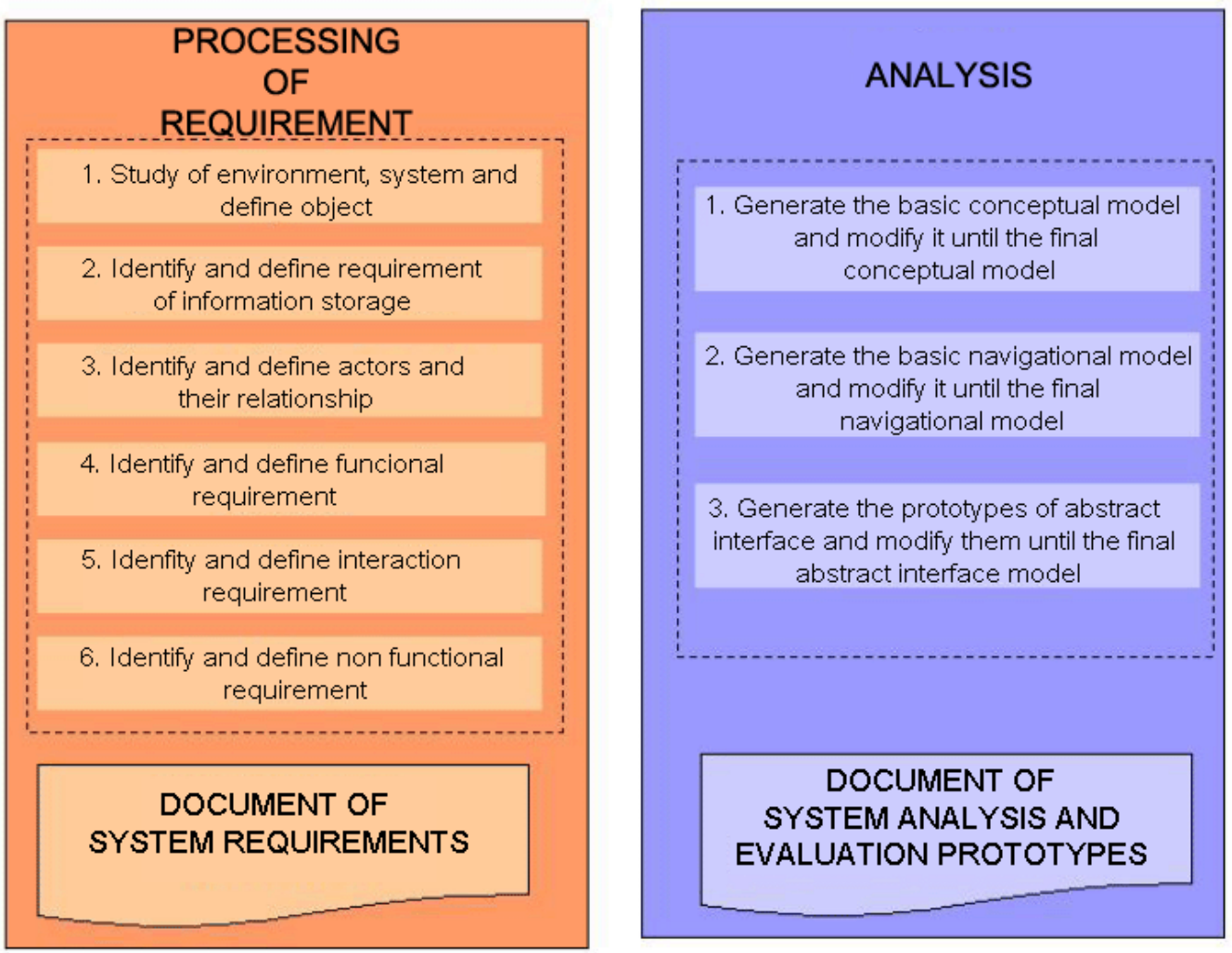
Introduction

- Grid portals make the work of the scientist lighter.
- Grid portals are an excellent approach to deliver to end user the capabilities provided by Internet-based Grids of computers.
- There are two issues to know before build a Grid portal.

Introduction

- Different methodologies for defining a web system can be used.
- The usefulness of standardized modelling approaches.
- Navigational Development Technique (NDT)

NDT (II)

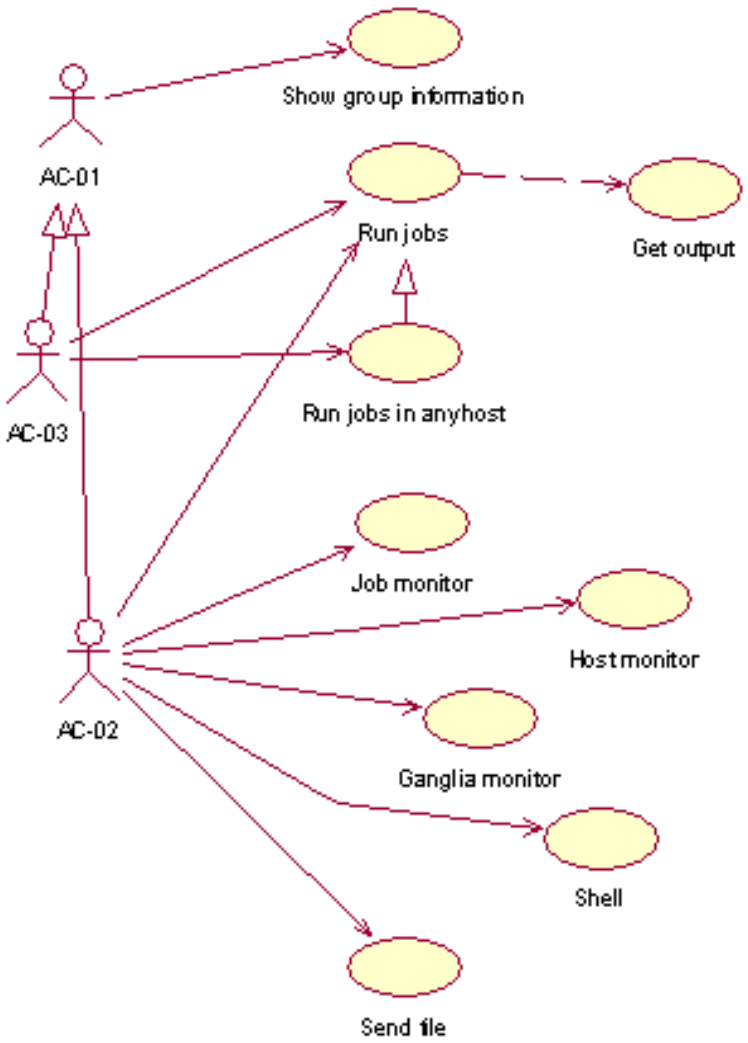

PROCESSING OF REQUIREMENT
1. Study of environment, system and define object
2. Identify and define requirement of information storage
3. Identify and define actors and their relationship
4. Identify and define funcional requirement
5. Idenfity and define interaction requirement
6. Identify and define non functional requirement
DOCUMENT OF SYSTEM REQUIREMENTS
ANALYSIS
1. Generate the basic conceptual model and modify it until the final conceptual model
2. Generate the basic navigational model and modify it until the final navigational model
3. Generate the prototypes of abstract interface and modify them until the final abstract interface model
DOCUMENT OF SYSTEM ANALYSIS AND EVALUATION PROTOTYPES

System Requirements analysis

Main Requirements

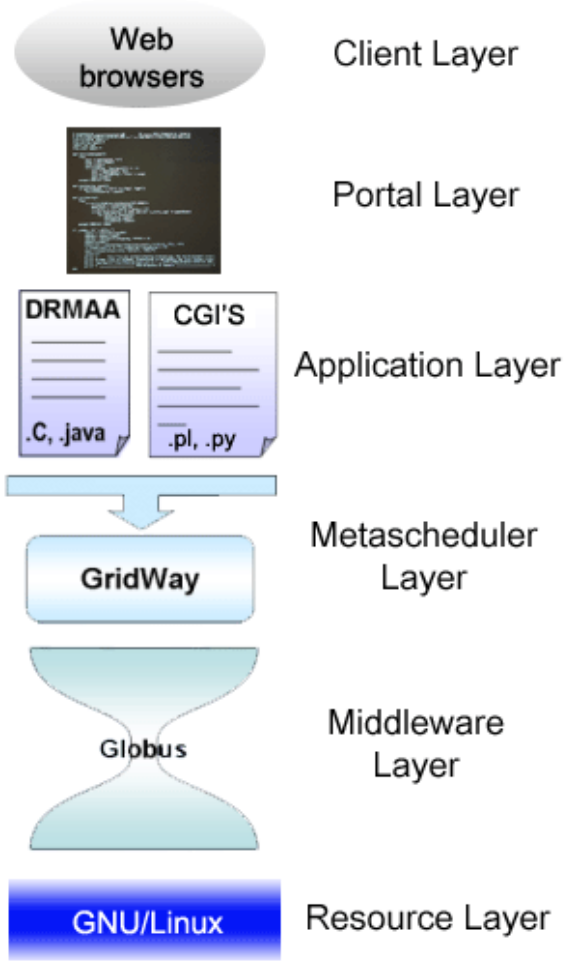
- The main requirements the system must fulfil are:
  - **Authentication**
  - **Security**
  - **Job selection and submitting**
  - **Monitoring**
    - **Jobs monitoring**
    - **Hosts monitoring**
    - **Grid (Ganglia) monitoring**
  - **Shell**
  - **Sending files**

NDT


Show group information
AC-01
Run jobs
Get output
AC-03
Run jobs in anyhost
Job monitor
Host monitor
AC-02
Ganglia monitor
Shell
Send file

SVO Grid Portal Architecture

Grid portal for Scientific Virtual Organizations (SVO)



Experiences

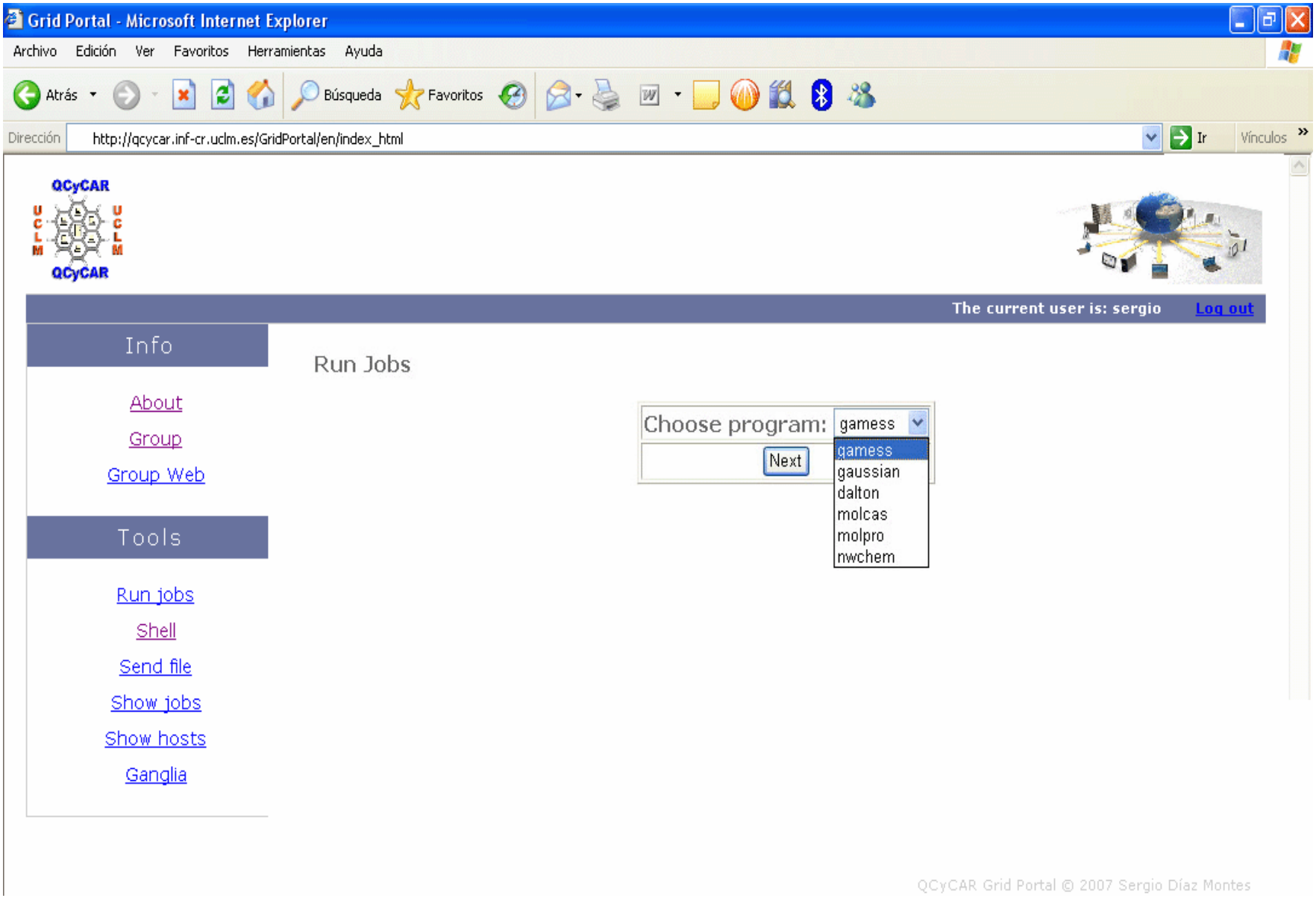
The Computational Chemistry Virtual Organization (C2VO) Grid Portal (I)

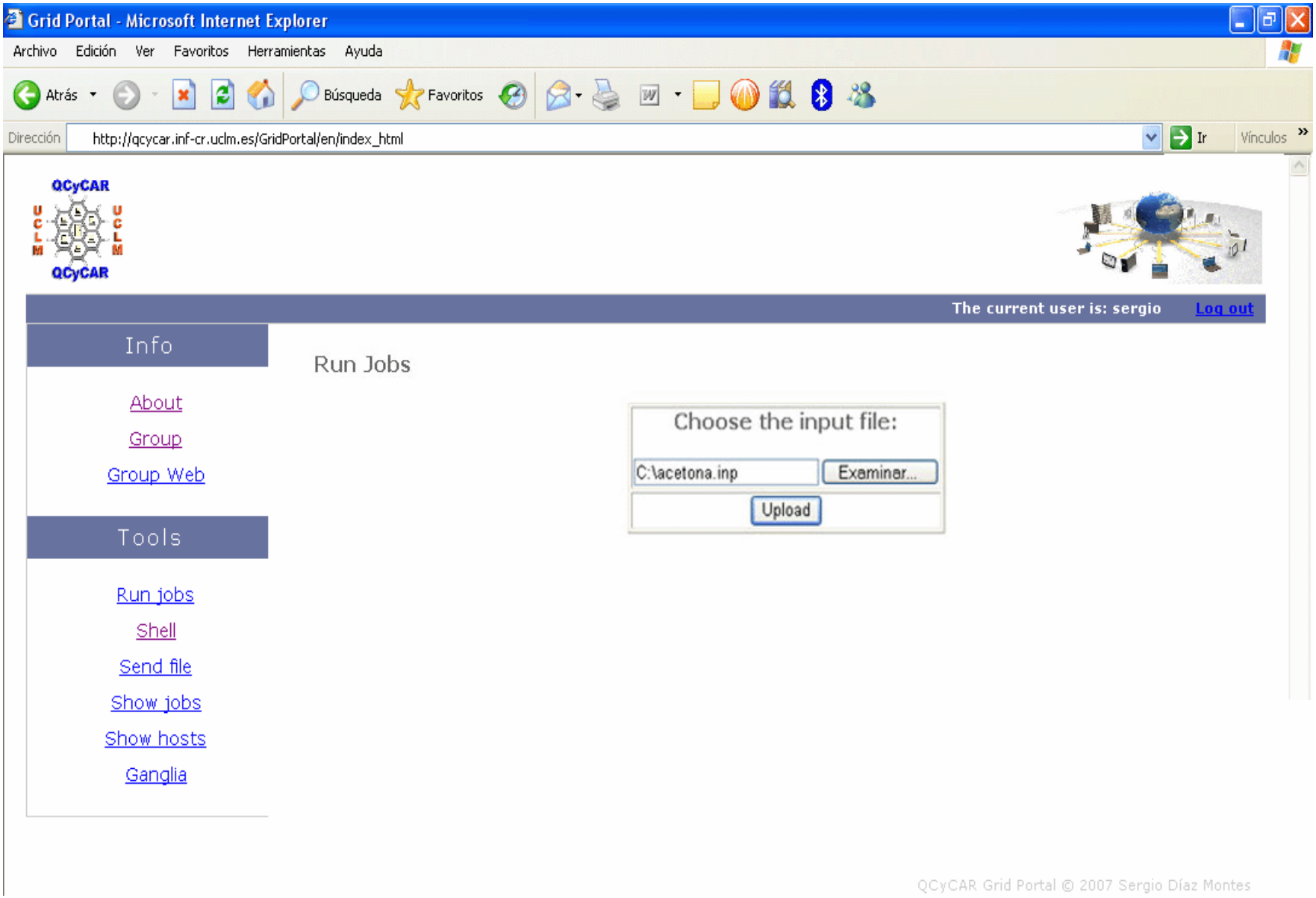
- There are a lot of Grid portals (GridSphere, GridPort).
- The main difference of the C2VO Grid portal.
- GridWay DRMAA API.
- Advantage with a metascheduler.

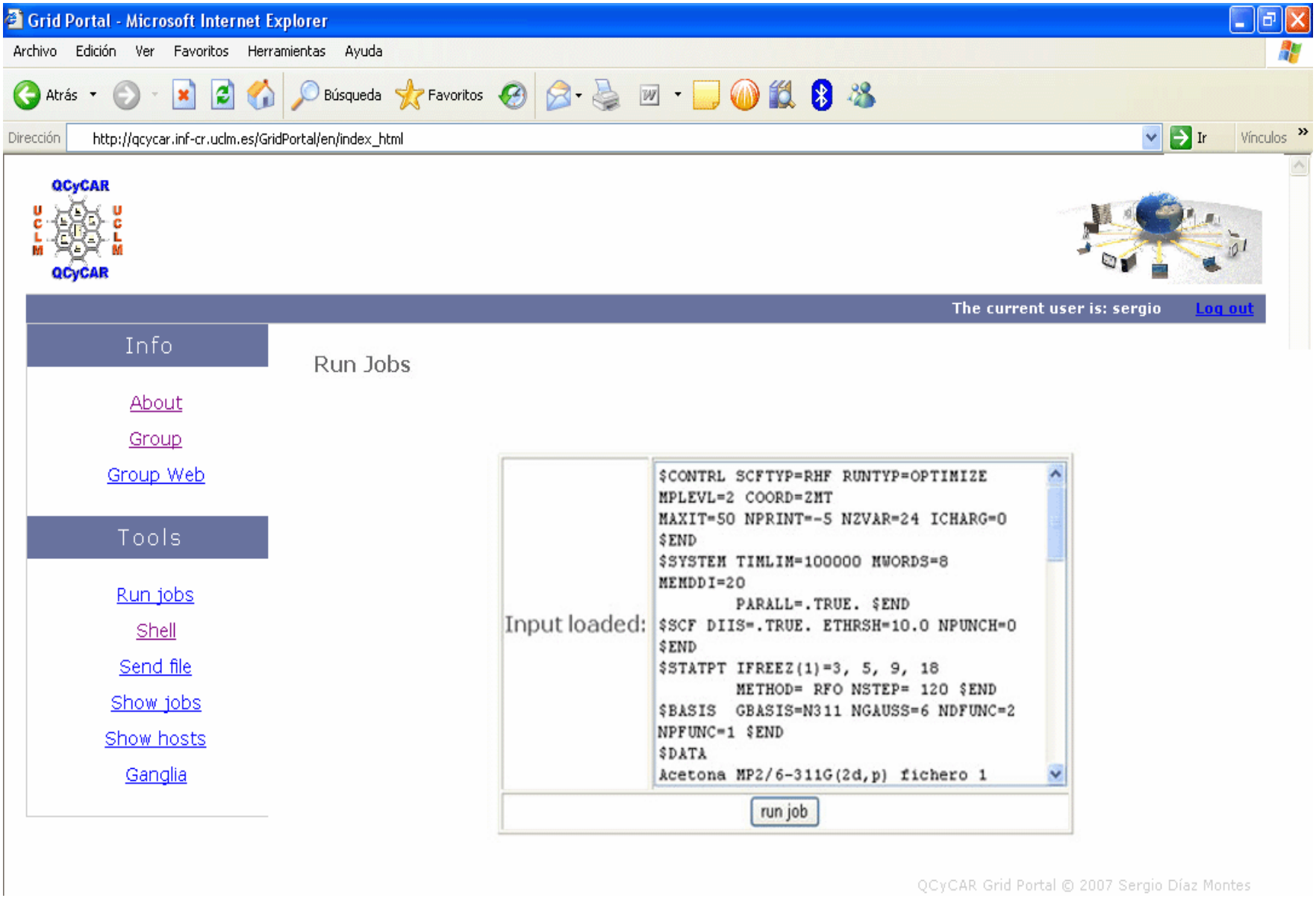
The Computational Chemistry Virtual Organization (C2VO) Grid Portal (II)

- As web server we have resorted to the open source web server Zope.
- The ZCGI Zope product.
- Zope is a framework allowing build web applications only with a web browser.
- MyProxy


Grid Portal - Microsoft Internet Explorer
Archivo Edición Ver Favoritos Herramientas Ayuda
Atrás Búsqueda Favoritos
Dirección http://qcycar.inf-cr.uclm.es/GridPortal/en/index_html
Ir Vínculos
QCyCAR
UCLM
QCyCAR
The current user is: sergio Log out
Info
About
Group
Group Web
Tools
Run jobs
Shell
Send file
Show jobs
Show hosts
Ganglia
Main Page
The Computational Chemistry and High Performance Computing group focuses in the development of Grid computing methods and techniques for high performance scientific applications. Our group is located at the Escuela Superior de Informática of the Universidad de Castilla la Mancha
QCyCAR Grid Portal © 2007 Sergio Díaz Montes


Grid Portal - Microsoft Internet Explorer
Archivo Edición Ver Favoritos Herramientas Ayuda
Atrás Búsqueda Favoritos
Dirección http://qcycar.inf-cr.uclm.es/GridPortal/en/index_html
Ir Vínculos
QCyCAR
UCLM
QCyCAR
The current user is: sergio
Log out
Info
About
Group
Group Web
Tools
Run jobs
Shell
Send file
Show jobs
Show hosts
Ganglia
Run Jobs
Choose program:
gamess
Next
gamess
gaussian
dalton
molcas
molpro
nwchem
QCyCAR Grid Portal © 2007 Sergio Díaz Montes


Grid Portal - Microsoft Internet Explorer
Archivo Edición Ver Favoritos Herramientas Ayuda
Atrás
Búsqueda
Favoritos
Dirección
http://qcycar.inf-cr.uclm.es/GridPortal/en/index_html
Ir
Vínculos
QCyCAR
UCLM
QCyCAR
The current user is: sergio
Log out
Info
About
Group
Group Web
Tools
Run jobs
Shell
Send file
Show jobs
Show hosts
Ganglia
Run Jobs
Choose the input file:
C:\acetona.inp
Examinar...
Upload
QCyCAR Grid Portal © 2007 Sergio Díaz Montes


Grid Portal - Microsoft Internet Explorer
Archivo Edición Ver Favoritos Herramientas Ayuda
Atrás Búsqueda Favoritos
Dirección http://qcycar.inf-cr.uclm.es/GridPortal/en/index_html
Ir Vínculos
QCyCAR
UCLM
QCyCAR
The current user is: sergio Log out
Info
About
Group
Group Web
Tools
Run jobs
Shell
Send file
Show jobs
Show hosts
Ganglia
Run Jobs
Input loaded:
$CONTRL SCFTYP=RHF RUNTYP=OPTIMIZE
MPLEVL=2 COORD=ZMT
MAXIT=50 NPRINT=-5 NZVAR=24 ICHARG=0
$END
$SYSTEM TIMLIM=100000 MWORDS=8
MEMDDI=20
PARALL=.TRUE. $END
$SCF DIIS=.TRUE. ETHRSH=10.0 NPUNCH=0
$END
$STATPT IFREEZ(1)=3, 5, 9, 18
METHOD= RFO NSTEP= 120 $END
$BASIS GBASIS=N311 NGAUSS=6 NDFUNC=2
NPFUNC=1 $END
$DATA
Acetona MP2/6-311G(2d,p) fichero 1
run job
QCyCAR Grid Portal © 2007 Sergio Díaz Montes

Aknowledgments

Aknowledgments

- **Organisms**
  - Junta de Comunidades de Castilla-La Mancha *(grant # PBI05-009)*
  - Ministerio de Educación y Ciencia *(grant # FIS2005-00293)*