



BIFI Applications in EDGeS

Alejandro Rivero(), Fermin Serrano*
al.rivero@gmail.com *fermin@bifi.es*

Instituto de  ocomputación
y  sica de sistemas complejos

EDGeS Meeting
October 2009 Mallorca Spain

Contents

- ❑ BIFI status
- ❑ Ibercivis overview
- ❑ Ibercivis – EDGeS connection
- ❑ Ibercivis applications running in EDGeS
 - ▶ MoU requirements
- ❑ Fusion Application
 - ▶ BIFI – EDGeS subcontract requirements
- ❑ Next steps

BIFI status

- BIFI is EDGeS subcontractor for fusion application
- BIFI leads Ibercivis project
 - ▶ Main Iberian BOINC multiproject site.
 - ▶ CETA and CIEMAT organizers too
 - ▶ Other organizers: CSIC (ES), RedIRIS (ES), FCCN (PT), Ucoimbra (PT), UMIC (PT)
- Ibercivis has signed MoU with EDGeS

Ibercivis Overview

- ❑ National (& iberian) initiative for volunteer computing and science dissemination
- ❑ Improvements vs other BOINC projects
 - ▶ Cluster approach easier access: Ibercivis shell
 - `./icivis_send_job nick priority app.jdl`
 - Option: queue management or self-managed
 - Still working on Workflow improvements.
 - ▶ Multiapplication project
 - ▶ Very long tasks management (continuity of jobs)
 - ▶ Distributed architecture
 - ▶ Optimized client
 - ▶ Dissemination and social components
 - www.ibercivis.net

Ibercivis Overview

□ Achievements

Users	15000
Cores connected per day	7000
Equivalent cores	1200
CPU time (14 months)	11 Millions hours
Research groups users	7+4

Applications in production phase: 7 projects

- ❑ Protein docking: CBMSO UAM-CSIC
- ❑ **Plasmas in ITER simulation: Ciemat-BIFI (runs in EDGeS)**
- ❑ Light in nanoscale: CSIC
- ❑ **Memory molecular structure (neurosim): CSIC (runs in EDGeS)**
- ❑ New magnetic materials: UCM, UNEX, BIFI
- ❑ Porous materials: IQFR CSIC
- ❑ Protein stability: UCoimbra

In alpha or beta phase:

- ❑ Nanoscale wires: Univ. Buenos Aires (Argentina)
- ❑ Neuronal networks: Univ. Extremadura
- ❑ Protein docking (GP 120): Univ. San Carlos (Guatemala)
- ❑ Montecarlo codes for braquitherapy: Hospital Puerta del Mar, Cadiz

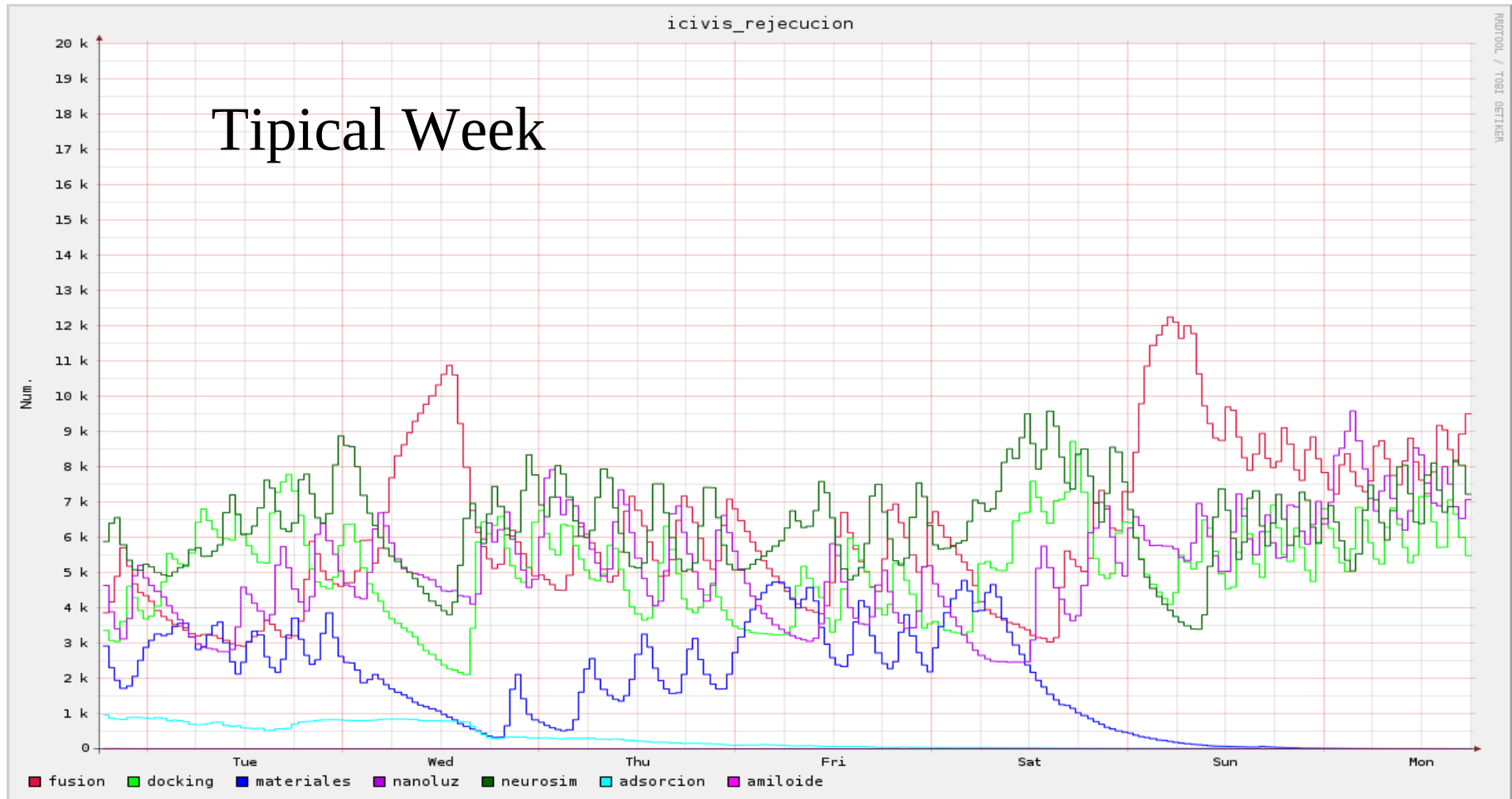
Open call for new applications close October 30



Ibercivis Overview



Typical Week



October 2009, Mallorca

BIFI Applications in EDGeS

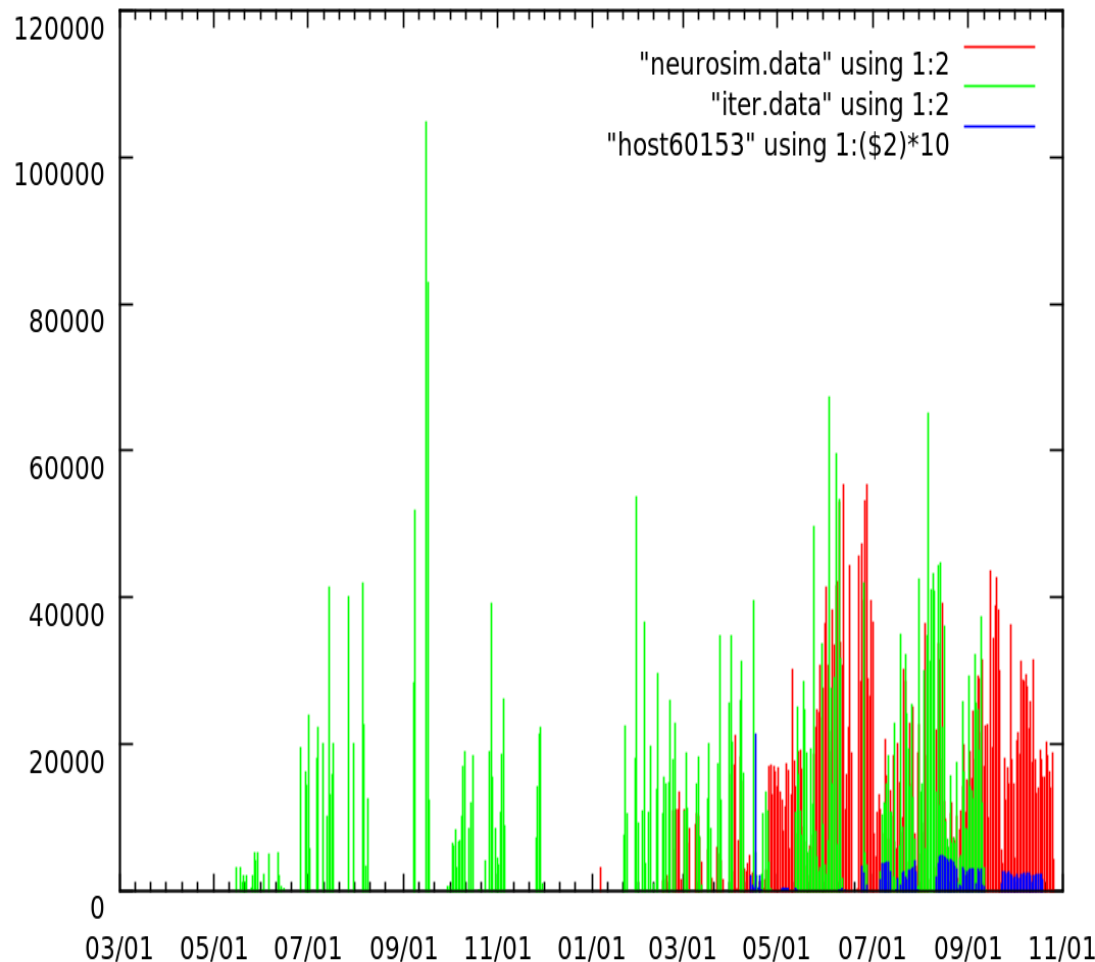
Ibercivis Overview



- Some jobs have HUGE workflows:
 - A job of Docking is 4 000 000 of independent subjobs
 - A job of Materiales is about 20 000 DAG subjobs of (up to) 20 segments each.
- Some researchers (eg Neurosim) prefer to use their AdHoc Workflow Management instead of our queue/jdl architecture
- (Anyway our DAG system is adHoc too, based on the assimilator)
- ITER/fusion runs shorter (30000 subjobs) workflows. Neurosim loops "collections"



Ibercivis – EDGeS connection



- EDGeS bridge and applications updated during this process (minor issues)
- DG2SG:
 - ▶ EDGeS bridge as a volunteer in Ibercivis
 - BOINC registration
 - Huge data files
 - Proxy and other renewals
 - ▶ BOINC ready applications don't need adaptation

Ibercivis – EDGeS connection



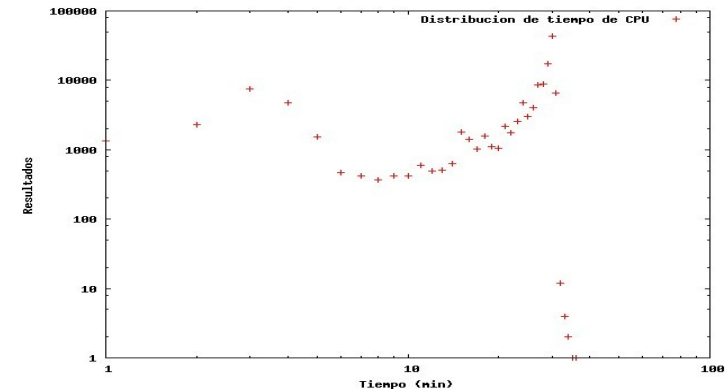
□ SG2DG:

- Being considered for production in the next phase of Ibercivis
 - Not a deliverable of EDGeS.
- ISDEP (fusion) app
 - already tested In EDGES testbed
 - candidate for validation
- BOINC “stand-alone” ready applications don't need adaptation to run in SG



Neurosim description

- ❑ Molecular Dynamics applications
 - ▶ Creation of statistical energy map of an aminoacid interacting with dipeptides and tripeptides for protein foldings
- ❑ 1 peptide = 1 run
- ❑ Executable size ~ 8MB
- ❑ Input files var ~200KB
- ❑ Output files ~200KB
- ❑ RAM needed ~50 MB
- ❑ Execution time ~5 min, variable, for each peptide
 - We group them up to 30 min.



Neurosim in EDGeS: DG2SG

- Neurosim ported to BOINC by ibercivis
 - Actually, it is GROMACS
 - ▶ Uses standard BOINC wrapper app.
 - ▶ runs in Ibercivis DG
- Runs in EDGeS VO SG
 - ▶ through EDGeS bridge
 - ▶ No porting or adaptation was needed

ISDEP description

- ❑ ITER device plasma simulation: 1 particle = 1 run
- ❑ Input files fixed ~80 MB
 - ▶ magnetic field configuration file
 - ▶ parameters file
 - ▶ measurement times
 - ▶ density, temperature and electric potential file
- ❑ Input files variables <1KB
 - ▶ configuration file
- ❑ Output files ~100K
 - ▶ configuration file
 - ▶ output
 - ▶ histogram
- ❑ RAM needed ~300MB
- ❑ Execution time ~30 minutes, variable, for each particle

ISDEP in EDGeS status: DG2SG

- ❑ ISDEP ported to BOINC in Zivis, then Ibercivis
 - ▶ Successful effort for Ibercivis and EDGeS
 - ▶ C application crosscompiled for Windows, Linux, Mac
 - ▶ BOINC API calls, templates fixed, validation mechanism
- ❑ ISDEP validated for us in Ibercivis
- ❑ Fusion WUs sets are available periodically so EDGeS bridge was configured to receive only fusion WUs
 - ▶ subcontract requirements
 - ▶ Problems with input files size, solved.
- ISDEP input files problem management:
 - Fusion WUs have modified their big input file management (soft link) because of EGEE jobs (187MB each)
 - Fusion WUs have reduced RAM requirements (1'5GB to 500MB)

ISDEP in EDGeS status: SG2DG

- ISDEP executed previously in EGEE
 - gLite version compiled
 - sh and jdl ready
 - Big input file transfer through SE
- ISDEP application has been deployed in EDGeS testbed
 - Compiled from Ibercivis sources
- Recreated set of Input Files for testing
- Fusion WUs have modified their big input file management (soft link ...)

ISDEP in EDGeS status: DG2SG

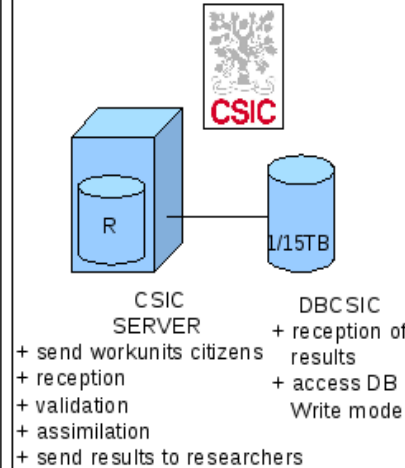
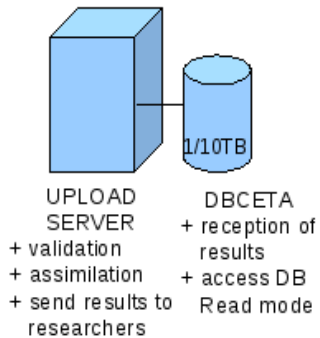
- ISDEP ported to Xtremweb
 - ▶ No activity in our side
 - ▶ First simulations launched and worked

Next Steps

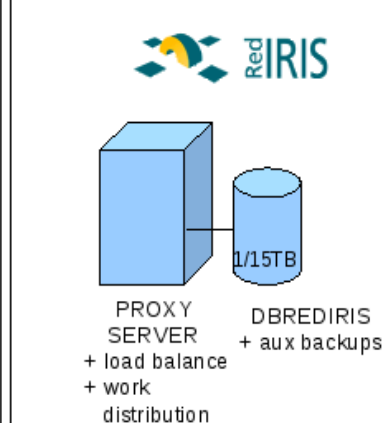
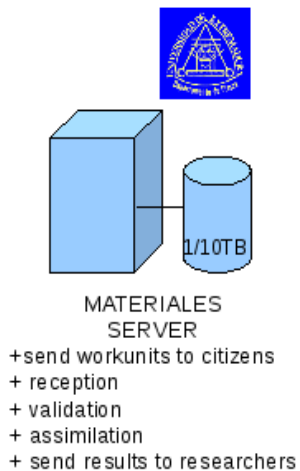
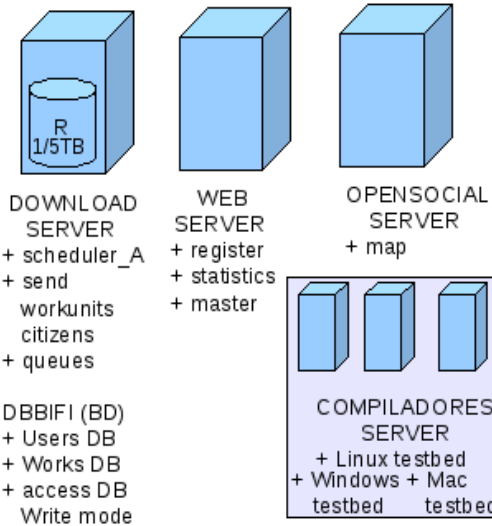
- ISDEP SG2DG validation
 - In process, almost done (Manuel)
 - Before November 15th
- Documentation required (ISDEP)
 - ▶ Deliverable report
 - Before December 15th
 - ▶ Tests documentation
 - ▶ DG2SG
 - Before December 1st
 - ▶ SG2DG
 - SZTAKI Team
- Documentation of Neurosim and other Ibercivis apps
 - ▶ Description and details already translated to English in the website

Thanks for your attention

IBERCIVIS INFRASTRUCTURE: HARDWARE RESOURCES DISTRIBUTION SEPT 09



Instituto de **L**icomputación
y **f**ísica de sistemas complejos



FCT
Fundação para a Ciência e a Tecnologia

