Mobyle @ RPBS

A web portal for structural bioinformatics and chemoinformatics.

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Introduction

RPBS Project

- Collaborative research in the field of structural bioinformatics
- Services related to protein structure

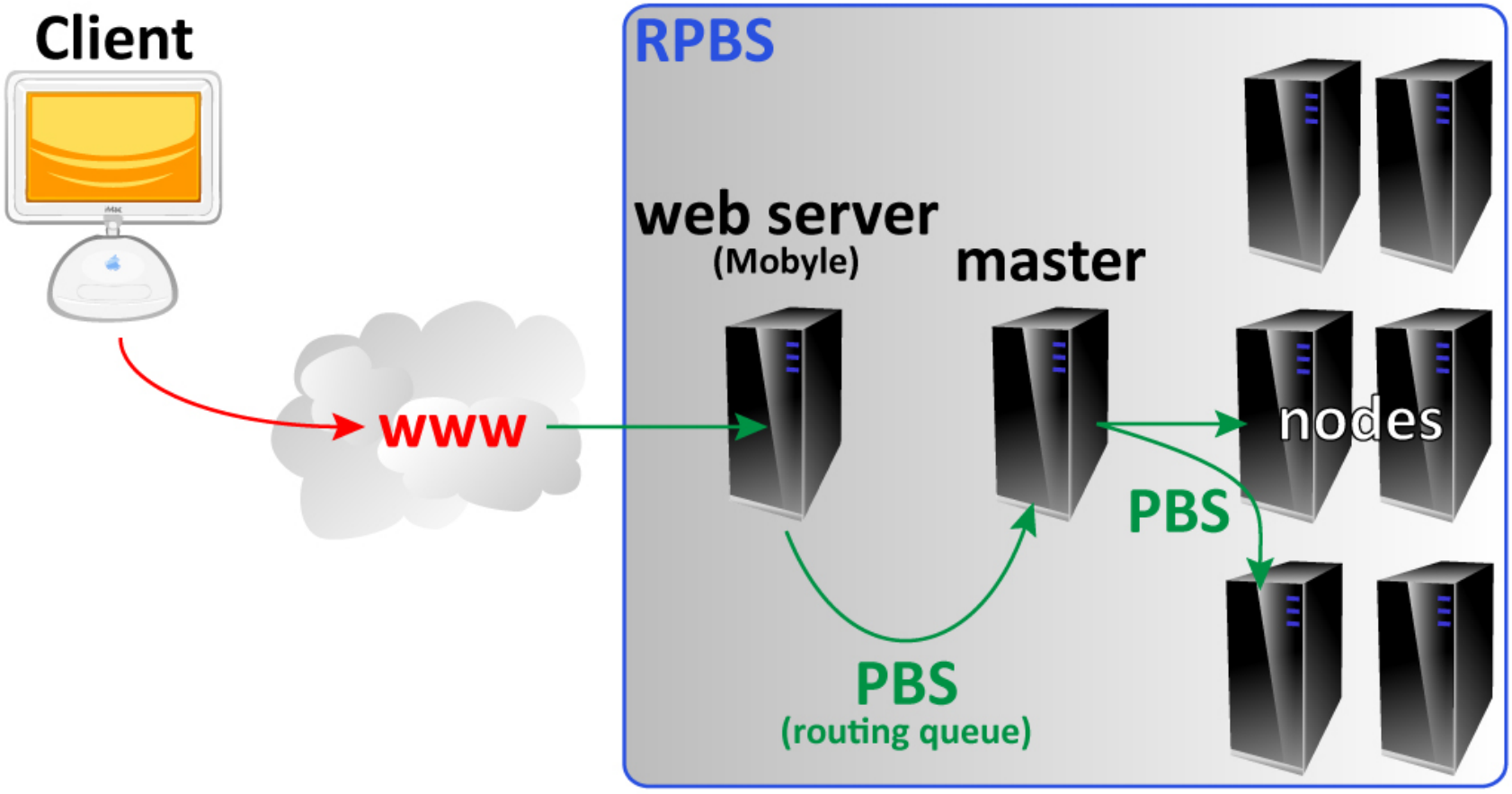
P-Server

- The first framework used at RPBS
- Mobyle inherited from some of its features
- All P-Server services moved to Mobyle@RPBS

Mobyle RPBS server

`http://mobyle.rpbs.univ-paris-diderot.fr`

Architecture



3D bioinformatics resource

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  - Relevant and RPBS-specific tools for protein structure **analysis** *(Stride, ASA, H-Bonds, PCE-pKa, PCE-pot, TEF, ...)*, **edition** *(side-chains substitution, add hydrogens, ...)*, **prediction** *(HCA, PSIPRED, SSpro, PEP-FOLD, MIR)*, **quality assessment** *(QMean)* ...

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MobyleNet

→ homology modeling pipeline

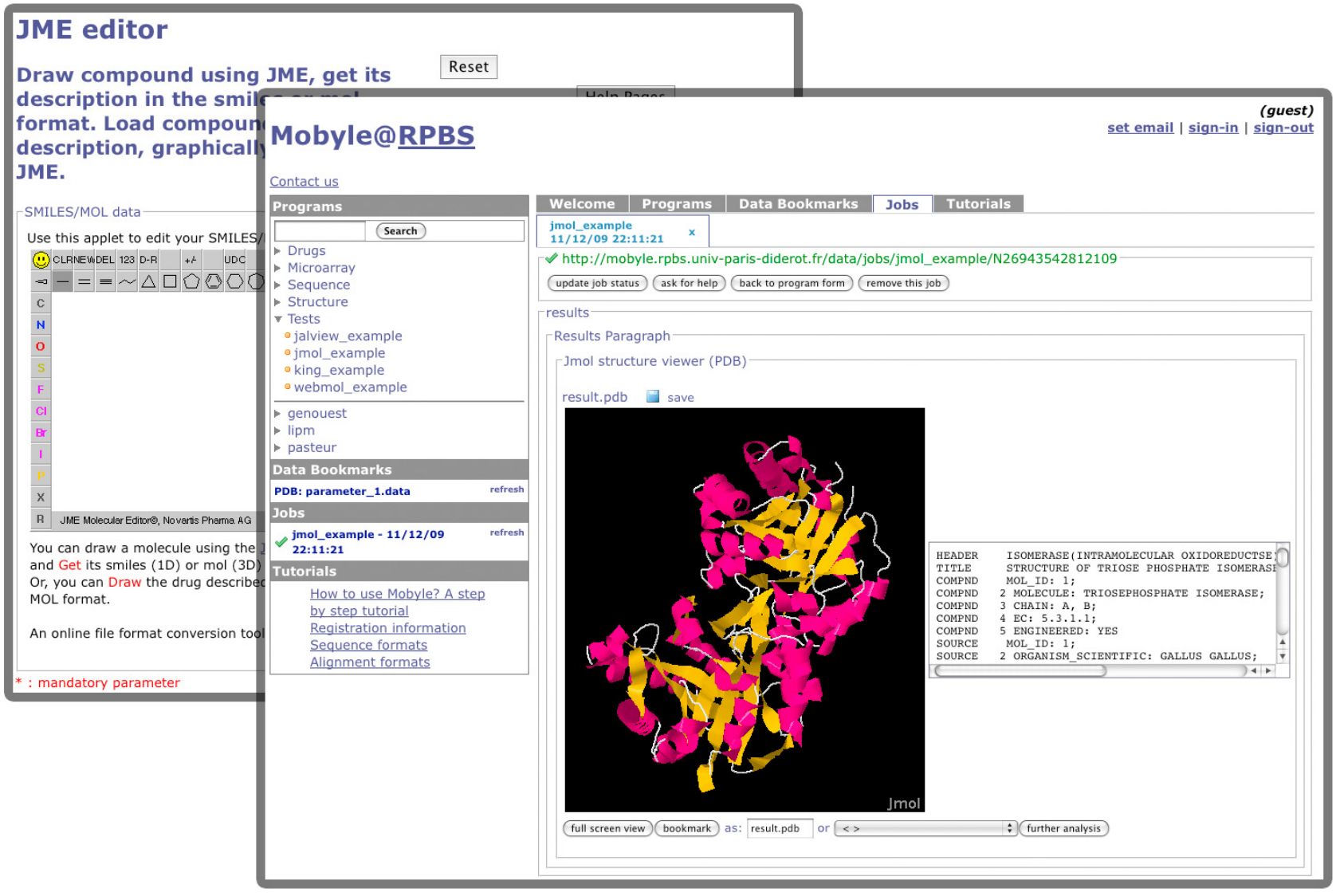
Datatypes

- Parameters datatype is the core of Mobyle (MobyleNet) pipelining capability
- MobyleNet common scheme for typing arguments. See : `http://mobylenet.rpbs.univ-paris-diderot.fr/doc/types.html`

Class	SuperClass	DataFormat
Sequence	-	FASTA, CLUSTAL, PIR, GDE, EMBL, GENBANK, SWISSPROT, PIR_3D
Alignment	-	
Structure	AbstractText	PDB, xyz, Mol2, smiles, sdf
...		

- There is no relevant converter for structural data, each parameter needs an accurate `<DataFormat>`

Java Applets



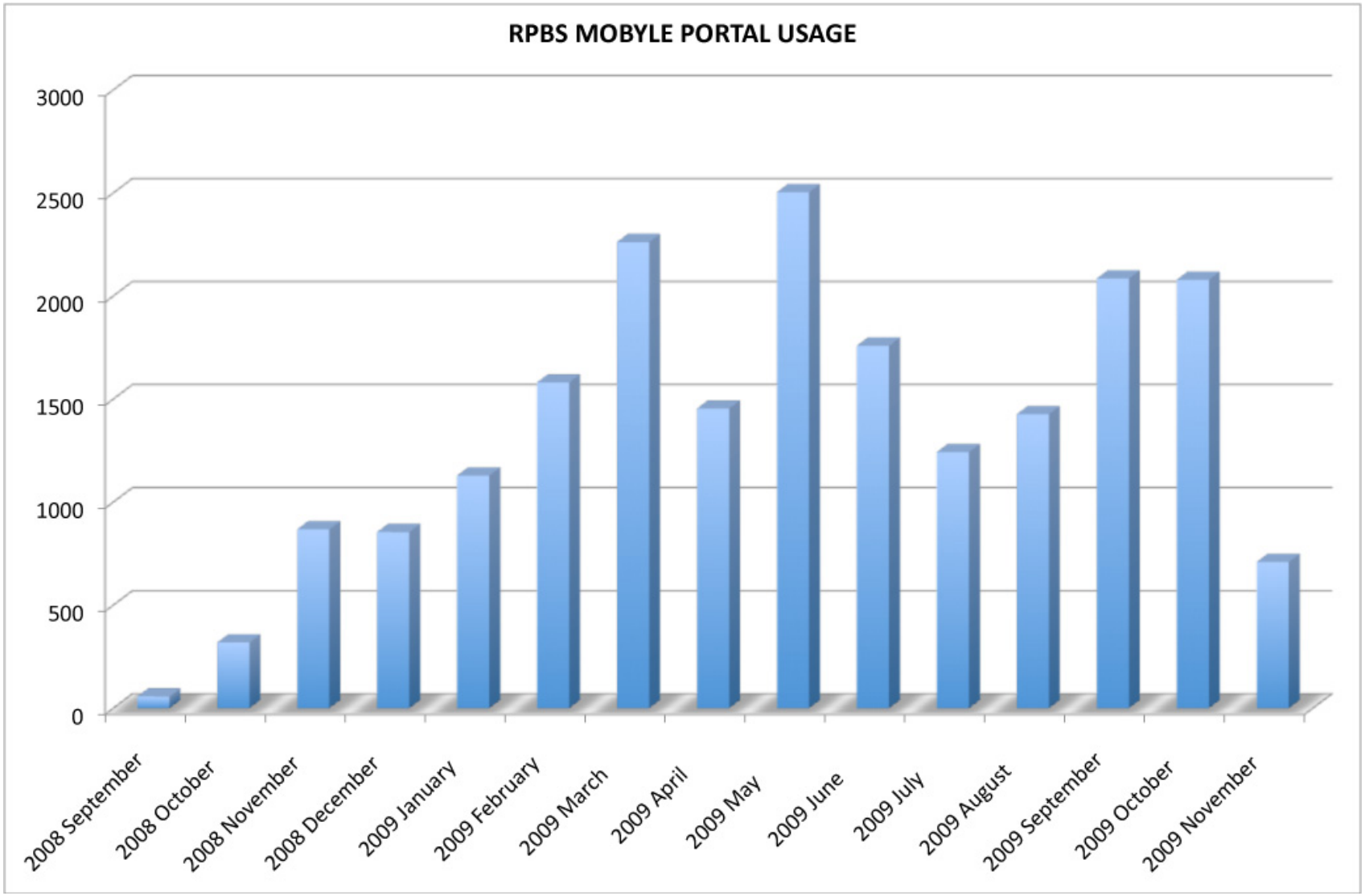
Java Applets

JMol applet example :

,,

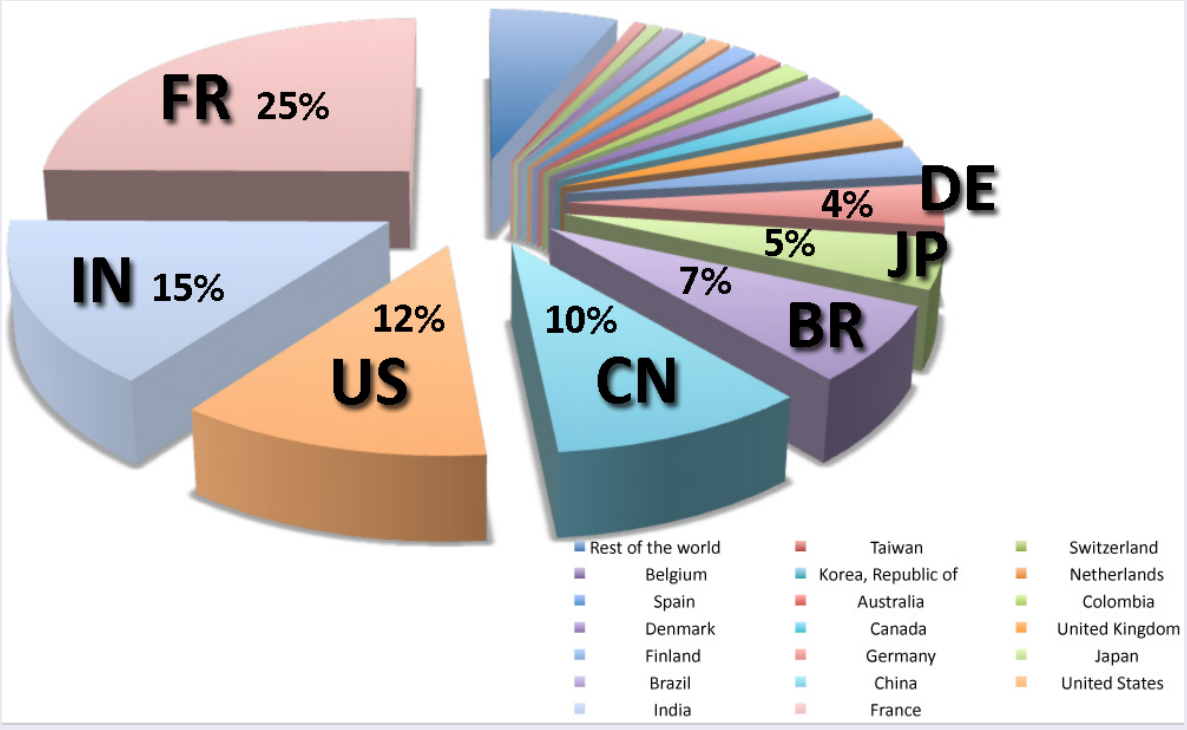
```
<interface>
  <table xmlns="http://www.w3.org/1999/xhtml" width="100%">
    <tr>
      <td width="50%">
        <applet code="JmolApplet" archive="/portal/applets/jmol/JmolApplet.jar"
            width="100%" height="450px">
          <param name="progressBar" value="true"/>
          <param name="load" value="$resultfile"/>
        </applet>
      </td>
      <td width="50%">
        <object xmlns="http://www.w3.org/1999/xhtml" type="text/plain" data="$
            resultfile" height="250px"/>
      </td>
    </tr>
  </table>
</interface>
```

Usage


RPBS MOBYLE PORTAL USAGE
3000
2500
2000
1500
1000
500
0
2008 September
2008 October
2008 November
2008 December
2009 January
2009 February
2009 March
2009 April
2009 May
2009 June
2009 July
2009 August
2009 September
2009 October
2009 November

Usage

Jobs location (2009/09 to 2009/11)



Stats

- Around **20000 jobs** launched since september 2008 from more than **5000 different locations**
- More than **5000 jobs since september 2009**
- **France** represents only **25%** of the jobs


B. Néron, H. Ménager, C. Maufrais, N. Joly, J. Maupetit, S. Letort, S. Carrere, P. Tuffery, and C. Letondal.
Mobyle : a new full web bioinformatics framework.
Bioinformatics, 25 :3005–3011, Nov 2009.


J. Maupetit, P. Derreumaux, and P. Tuffery.
PEP-FOLD : an online resource for de novo peptide structure prediction.
Nucleic Acids Res., 37 :498–503, Jul 2009.


O. Sperandio, M. Petitjean, and P. Tuffery.
wwLigCSRre : a 3D ligand-based server for hit identification and optimization.
Nucleic Acids Res., 37 :W504–509, Jul 2009.