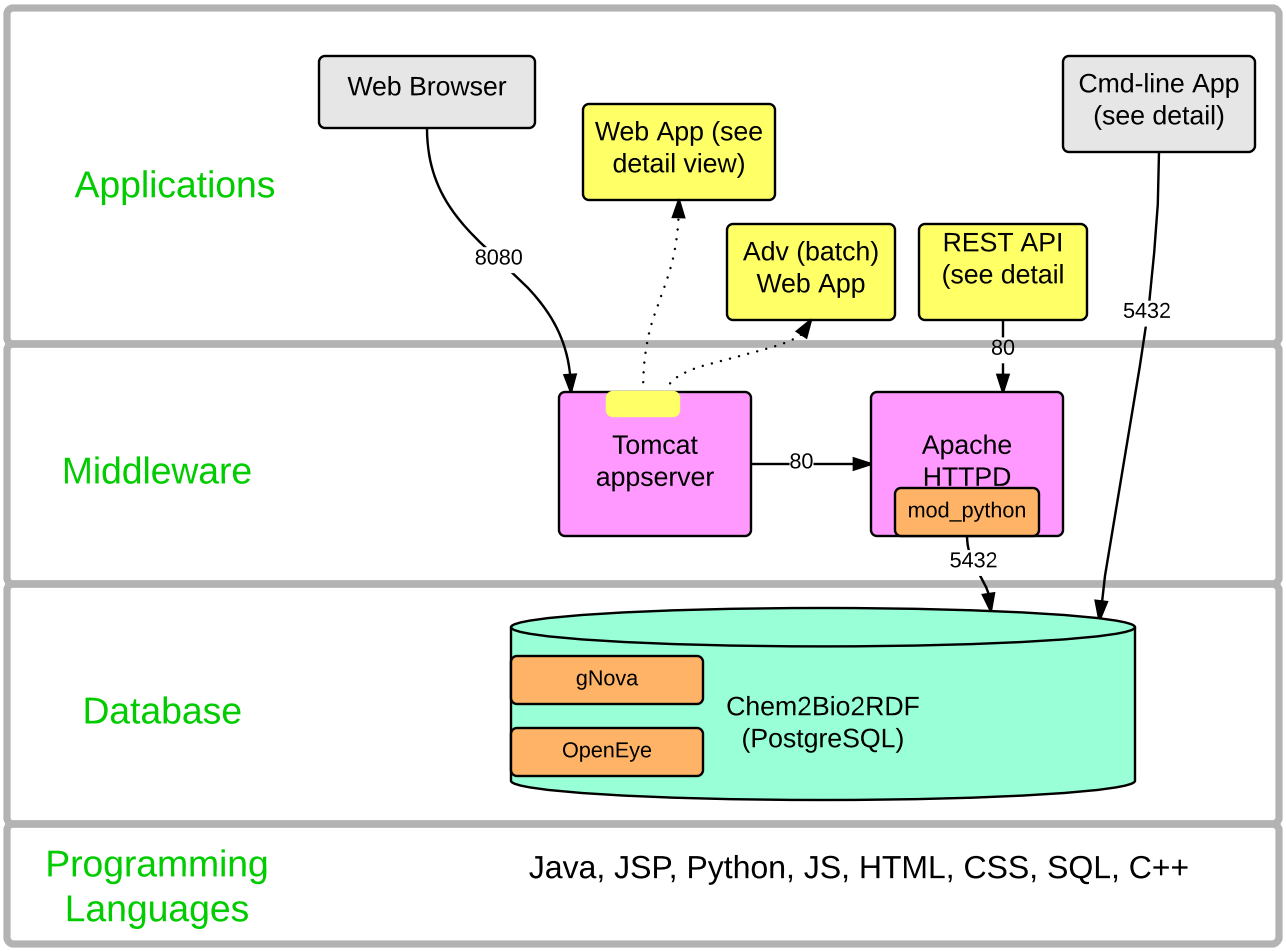
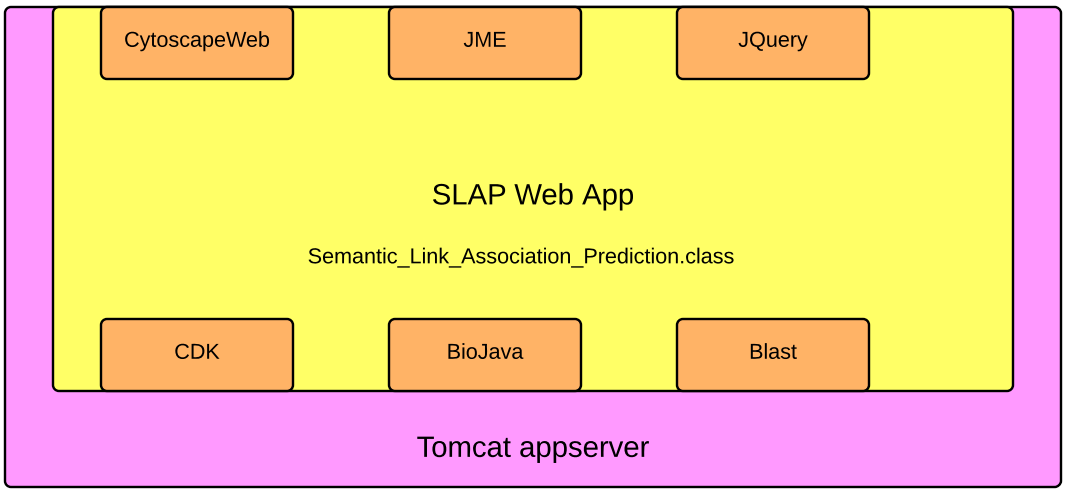
SLAP Architecture (runtime)

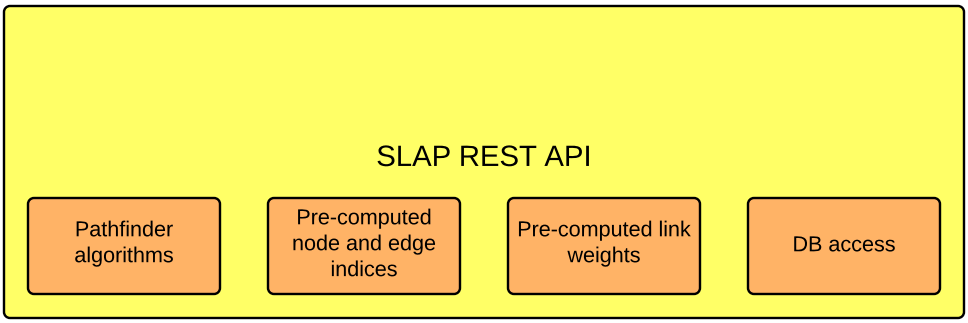


SLAP Web App detail



- Installed at /usr/share/tomcat5/webapps/slap
- index.jsp is home page. References class "Semantic_Link_Association_Prediction" and others.
- See WEB-INF/web.xml for all servlet URLs.
- WEB-INF/classes/Prediction/Semantic_Link_Association_Prediction.class
- Java calls SLAP REST API.
- Subdir "swf" contains CytoscapeWeb.swf
- JME.jar is Java Molecular Editor
- WEB-INF/lib contains several libraries, perhaps not all required at runtime.

SLAP REST API detail



- Served by Apache HTTPD via mod_python (for speed, "SetHandler cgi-script" should also work)
- Installed at /var/www/html/rest/Chem2Bio2RDF/slap
- .htaccess key lines:
  - SetHandler mod_python
  - PythonHandler prediction1
- Note that use of .htaccess reduces performance.
- See also: /etc/httpd/conf.d/python.conf (mod_python config).
- prediction1.py imports SLAP codes: odbc6, ppDrugTargetPrediction1, ppPairPrediction2, pathfinder_rank5
- Python packages: pp, psycopg2, xml.dom.minidom, SOAPpy, SPARQLWrapper
- odbc6.py contains SQL to access Chem2Bio2RDF DB.
- Example URIs:
  - /rest/Chem2Bio2RDF/slap/5591:PPARG

Path-Pattern finding, weighting, statistics

(batch pre-processing, not runtime)

- Also from cheminfov:/var/www/html/rest/Chem2Bio2RDF/slap.
- pathfinder_m.py
- pathfinder_rank5.py (runs findPath_m)
- findPath_m (compiled binary, no source)
- pathfinder_m (copy of findPath_m, same checksum)
- pathfinder_rank_advanced.py (experimental?)
- Note that pathfinder_m.py 2010, pathfinder_rank5.py 2011, newer version.
- pathfinder_rank5.py requires subdir "Dicts" files:
  - node2id.txt
  - pair_weight.txt
  - pattern_distribution.txt
- Some files and components may be needed to generate dict files:
  - PreProcess?
  - Virtuoso?

SLAP Command-line App Detail

- ppPairPrediction_local.py is command line application for running SLAP.
- Requires package pp (Parallel Python)
- Postgresql via odbc6.py and psycopg2
- odbc6.py uses NCBI Entrez for getGeneByNameNIH() and retrieveCIDsByNameDrugbank().
- Input file list of compound-protein pairs.

```
cheminfov$ ppPairPrediction_local.py
ERROR: Syntax: ppPairPrediction_local.py ifile ofile
```

Example input file:

```
4737    CHRNA9
4737    CHRNB2
4737    CHRNB3
4737    CHRNB4
4737    CLK1
4737    CLK3
4737    CNR1
4737    CNR2
4737    CPA1
4737    CPB1
4737    CPT1A
```

SLAP DB

- PostgreSQL database, access via ODBC.
- Subset of Chem2Bio2RDF is required for SLAP, "SLAPDb".
- Based on review of SQL in REST API Python code, required tables:
  - c2b2r_chembl_08_target_dictionary
  - c2b2r_chemogenomics
  - c2b2r_compound_new
  - c2b2r_drugbankdrug_042011
  - c2b2r_Gi2UNIPROT_new
  - c2b2r_GENE2UNIPROT
  - c2b2r_HGNC
  - c2b2r_omim_disease
  - pubchem_compound
- Tables renamed (with schema):
  - c2b2r.chembl_08_target_dictionary
  - c2b2r.chemogenomics
  - c2b2r.compound_new
  - c2b2r.drugbankdrug
  - c2b2r.gi2uniprot
  - c2b2r.gene2uniprot
  - c2b2r.hgnc
  - c2b2r.omim_disease
  - c2b2r.pubchem_compound