

# OPAL Dashboard with DUCKLING Tools

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# Proposed Project

- Develop a Dashboard Similar to the Opal Dashboard located @ [ws.nbcrc.net/opal2](http://ws.nbcrc.net/opal2), and add user control by using duckling's tools.
- The Dashboard should show all the applications (services) deployed on NBCR web server ([ws.nbcrc.net](http://ws.nbcrc.net))
- Based on each application's metadata, dashboard should Automatically Generate User Interfaces (forms), and collect information upon submit.
- Collected information will be submitted to that application's Service URL, and request to run job based on those information.

## Proposed Project (cont'd)

- As in return from the service, Dashboard will get a Output URL and store it into database reference it with current user.
- Users can see previous job submissions in the Job History page.

# Dashboard via Duckling

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### 欢迎使用Duckling协同工作环境！

**2010年3月17日, Duckling开源啦！**

**Duckling协同工作环境研究中心**

支持e-Science的协同工作环境（Duckling）开源软件是专为科研团队提供的综合性的资源共享和协作平台。面向新型科研活动方式的需求，通过协同工作环境核心工具集和在其门户平台框架（支持Portlet框架）下开发的各类学科应用插件，集成网络环境中的硬件、软件、数据、信息等各类资源，为科研人员提供先进的信息化科研平台。用户可在该平台下按照portlet规范开发特定的插件应用。

如果您有使用中的疑惑，请访问[使用帮助](#)。

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**【支持服务：010-58812345 [vlab@cnic.cn](mailto:vlab@cnic.cn)】**

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# Login & Register Page

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### Sign in

Username   
ⓘ Please Enter an Username

Password   
 [Forgot your password](#)

### Register if don't have an account!

Username \*  ⓘ Please Enter an Email

Password \*  ⓘ Please enter password

Retype \*  ⓘ please confirm password  
Password

Fisrt name \*  ⓘ Please Enter Your First Name

Middle name  ⓘ optional

Last name \*  ⓘ Please Enter Your Last Name

Company  ⓘ optional

Job Title  ⓘ optional

Cell Phone  ⓘ optional

# Home Page

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### Menu

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### Home Page

**Welcome to Dashboard!**

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-  [Collaboration Environment Research Center \(CERC\)](#)
-  [Duckling](#)
-  [The Opal Toolkit](#)

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# Application List Page

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### Service List

ALL	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	#
<a href="#">APBS 1.2.1b</a>											<a href="#">GLAM2SCAN_4.6.1</a>																<a href="#">MEMECHIP 4.6.1</a>
<a href="#">APBS-Parallel 1.2.1</a>											<a href="#">GLAM2_4.6.0</a>																<a href="#">MEME_4.6.0</a>
<a href="#">Autodock4.2.1</a>											<a href="#">GLAM2_4.6.1</a>																<a href="#">MEME_4.6.1</a>
<a href="#">Autodock_4.0.1</a>											<a href="#">GOMO_4.6.0</a>																<a href="#">PDB2PQR 1.7.0</a>
<a href="#">Autogrid_4.0.1</a>											<a href="#">GOMO_4.6.1</a>																<a href="#">Prepare GPF 1.5.4</a>
<a href="#">Autogrid_4.2.1</a>											<a href="#">MAST_4.6.0</a>																<a href="#">Prepare_receptor_1.5.4</a>
<a href="#">Env test</a>											<a href="#">MAST_4.6.1</a>																<a href="#">SPAMO_4.6.0</a>
<a href="#">FIMO_4.6.0</a>											<a href="#">MCAST_4.6.0</a>																<a href="#">SPAMO_4.6.1</a>
<a href="#">FIMO_4.6.1</a>											<a href="#">MCAST_4.6.1</a>																<a href="#">TOMTOM</a>
<a href="#">GLAM2SCAN_4.6.0</a>											<a href="#">MEMECHIP 4.6.0</a>																<a href="#">TOMTOM</a>

# Application's metadata

- Application's metadata are requested from application's service URL by using Opal2's function :  
`AppServicePortType.getAppConfig();`
- There are four types of application metadata:
  - Flag: Chackbox.
  - Tagged Parameter: Parameters with tag id.
  - Untagged Parameter: Parameters without tag id.
  - Groups: Specify groups for the above three type, a group may exclusive, in this case, we need to add ratio button for user to choose.



# Application Page (metadata)

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### Autodock\_4.0.1's Submit Form Back

**Ungrouped input fields**

<input type="checkbox"/>	Use old PDBQ format, charge q in columns 55-61
<input type="checkbox"/>	Keep original residue numbers
<input type="checkbox"/>	Ignore header-checking
<input type="checkbox"/>	Parse the PDBQ file to check torsions, then stop
Parameter Filename*	<input type="button" value="Choose File"/> No file chosen
Name of the log file*	<input type="text"/>
Ligand PDBQT file*	<input type="button" value="Choose File"/> No file chosen
URL where to fetch the MAP files*	<input type="text"/>

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# Application Page (metadata)

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**PDB2PQR 1.7.0's Submit Form** Back

**Input file to be used (choose one of the two options)\***

The PDB input file (for testing you can download <http://www.rcsb.org/pdb/files/1a1p.pdb>) Choose File no file selected

The ID to use to retrieve the input file from the PDB archive (for testing use '1a1p')

**Other required parameters\***

The forcefield to use -- currently AMBER, CHARMM, PARSE, and TYL06 are supported.\*:

AMBER  
 CHARMM  
 PARSE  
 TYL06

The desired output name of the PQR file to be generated\*

**Output naming schema to be used**

Instead of using the standard canonical naming scheme for residue and atom, use names from the given forcefield:

AMBER  
 CHARMM  
 PARSE  
 TYL06

**Additional optional command-line arguments from the extensions directory are**

Print the per-residue backbone chi angle to {output-path}.chi

Print the per-residue backbone phi angle to {output-path}.phi

Print the per-residue phi and psi angles to {output-path}.rama for Ramachandran plots

Print the per-residue backbone psi angle to {output-path}.psi

Print a list of hydrogen bonds to {output-path}.hbond

# Application Page (basic)

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### GOMO\_4.6.0's Submit Form Back

Insert command line here:	<input type="text"/>
	<a href="#">See help for command detail</a>
Choose input file:	<input type="button" value="Choose File"/> No file chosen
	<input type="button" value="Choose File"/> No file chosen
	<input type="button" value="Choose File"/> No file chosen
	<input type="button" value="Choose File"/> No file chosen

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# Job Submission

- There are two basic information we need to send to server:
  - Command
  - Uploaded Files
- Service will return a Job ID in return of job request, based on ID, we can go to [ws.nbcr.net/jobid](http://ws.nbcr.net/jobid) (output URL) to get all the uploaded files, and job output file(result).

# Job Result Page

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### Job Submitted

Application Name	PDB2PQR 1.7.0	Application ID	app1313676869882
Output URL	<a href="http://ws.nbc.net/app1313676869882">http://ws.nbc.net/app1313676869882</a>	Submission Time	2011-08-18 22:14:30
Generated command	--verbose --ff=AMBER 1a1p output.pqr		

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# Job History Page

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### List of Job Output

AppName	AppID	Date	Command
PDB2PQR 1.7.0	<a href="#">app1313676936061</a>	2011-08-18 22:15:36	--verbose --ff=AMBER 1a1p output.pqr
TOMTOM	<a href="#">app1313676978178</a>	2011-08-18 22:16:18	--uploaded rgb.txt pearson evaluate 0.5 README.txt p
Autodock_4.0.1	<a href="#">app1313677039678</a>	2011-08-18 22:17:20	-p change.txt -l logfile farsi.txt urls
MCAST_4.6.0	<a href="#">app1313677103618</a>	2011-08-18 22:18:23	-p-tresh eval.txt
GLAM2_4.6.1	<a href="#">app1313677205348</a>	2011-08-18 22:20:05	-p-tresh eval.txt

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# Database

- There are three tables for database dashboard:
  - Users: contains information about user including email, name, company, job title, cell phone number, register date.
  - Jobs: contains all the job submission including job id, output URL, submit date, command, reference to Users.
  - Services: contains information about services including service name, service URL, service usage.
- There are also Duckling database to save user email, and password...

# What I have Learned

- Spring MVC Portalet
  - Easier and More futures than Struct.
- MySQL Database
- Jquery and CSS
- Duckling (installation)
- Setup Linux Server.
- Myeclipse on Win7.



# Things can be improved

- Validation for metadata application page.
- Save application metadata into database (MongoDB)
- User Control page for admin (userlevel = 0).
- A page where user can change their information including password.
- Register email validation by umt, not dashboard's database.
- Add more duckling tools.

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