EXPERIENCES FROM SHARING AN AUTODOCK VINA WORKFLOW FOR VIRTUAL SCREENING USING THE SHIWA WORKFLOW REPOSITORY

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ER-flow

See previous presentation by Kitti 😊
Application: Autodock Vina

• **Purpose**
  – Drug discovery
  – Molecular docking
  – Virtual screening

• **Qualities**
  – Multi-core capabilities
  – High performance
  – Enhanced accuracy
  – Ease of use

• Experiments demands large computing power
Vina @ Westminster

- Collaboration by researchers from School of Life Sciences and School of Electronics and Computer Science
- Composed workflow using the WS-PGRADE workflow system and science gateway framework
- Enabled the researchers to execute large scale virtual screening experiments from a high level science gateway interface
Vina @ AMC

• Scientists in the department of Medical Biochemistry also use Autodock Vina for virtual screening experiments
• Virtual screens of large databases are used as a starting point to identify small molecules that can interact with proteins and modulate activity
• Potential targets are further evaluated using conventional biochemical assays
• With the growth of databases, running their experiments on their local infrastructure became more and more challenging due to long computation times
New collaboration

- Approached the e-BioScience team
- Experience with running Next Generation Sequencing and Medical Imaging applications on EGI through their e-BioInfra Gateway
- ER-flow and SCI-BUS partner
Westminster Workflow

• The workflow was originally supported to run on the BOINC-based local desktop grid
• Later ported to the public volunteer computing resources of EDGeS@home
• Published in the SHIWA Workflow Repository
  – Enabling other researchers to execute the workflow directly on the SHIWA Simulation Platform
  – Allowing to download and customize the workflow according to their requirements.
Workflow: PublicAutoDockVina112 | Engine: WS-PGRADE(3.4.5) | Implementation version: 1.00

Graph

Implementation summary

Title: Public AutoDock Vina 1.1.2 - Virtual screening of a library of ligands
Workflow: PublicAutoDockVina112
Engine: WS-PGRADE(3.4.5)
Version: 1.00
Status: new
Language: WS-PGRADE
Licence: Apache License 2.0
Definition: workflow.xml
Keywords: AutoDock, virtual screening, receptor, protein, ligand, molecule docking
Created: 06.11.12 0:00, Modified: 07.11.12 14:08

Description: This workflow performs virtual screening of molecules using version 1.1.2 of AutoDock Vina. It docks a library of small ligands on a selected receptor molecule. For further information, please download and contact the README file.
Workflow details

• Breaking up in work units to allow for parallelization

• Wrapper around binaries

• Merging the results and selecting the N best results
Implementation @ AMC

• Workflow was imported from the SHIWA Repository into the AMC portal

• Modified for the local usage scenario
  – PBS
  – gLite
Porting issues

• SHIWA Import vs “Download + Upload”

• Strong coupling to infrastructure (theory vs practice)

• “Missing” component reverse-engineering
The last mile
End-user view WS-PGRADE
Customized Portlet (beta)
Interactive view
Conclusions

• Workflows for developing, describing, executing and sharing science works!

• Devil is in the details!

• Developers vs Users

• Generic vs Customized interface?