Enhancing the Galaxy Tool Shed

http://usegalaxy.org/toolshed
http://wiki.galaxyproject.org/Tool%20Shed

Greg Von Kuster
The Galaxy Team
The Galaxy Tool Shed is an App Store

- The Tool Shed is a fully functioning, online App Store when used in conjunction with the enhanced Galaxy features that complement it
- The Tool Shed enables installation of Galaxy utilities into any web accessible Galaxy environment
- The Tool Shed uses mercurial repositories to contain Galaxy utilities
- The Tool Shed enables acquisition of updates for Galaxy utilities installed into a Galaxy environment
What are Galaxy Utilities?

- **Tools** for data analyses
- **Data** (acquired using specialized Data Manager tools)
- **Custom Datatypes**
- **Tool Dependency** definitions
- **Repository Dependency** definitions
- **Exported Galaxy Workflows**

Additional utilities will be supported in the future
Tool Dependency Definitions

- A tool dependency definition is an XML file included in a Tool Shed repository named `tool_dependencies.xml`

- The file includes the recipe for installing and compiling all required tool dependencies into the Galaxy environment

- The dependencies framework supports defining dependencies that require other dependencies

- A specific dependency version will be installed only once, with any number of Galaxy utilities able to use it
Repository Dependency Definitions

- A repository dependency definition is an XML file included in a Tool Shed repository named `repository_dependencies.xml`.
- The file defines relationships to any number of repositories.
- Relationships at the repository level are defined as “simple”.
- Relationships at the repository contents level (Galaxy utilities) are defined as “complex”.
Order matters!

- Some tool dependencies may require other tool dependencies to be installed first
- Repository dependency definitions provide support for ordering the installation of the dependency hierarchy
Time matters too!

• Tool dependency definitions support relationships created for dependency compile time and for tool execution time
Options for installation

- Galaxy utilities can be installed using either a browser or the Galaxy API for the Tool Shed
An example

- Björn Grüning’s chemicaltoolbox
  [http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox](http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox) incorporates all of these features
## Dependencies of this repository

- **Repository dependencies** - This is a metapackage that will install several other tools.
  - **chemical_data_sources** revision 955783ed18f owned by bgruening
  - **molecule_datatypes** revision a1474892287e owned by bgruening
  - **package_numpy_1_7** revision ad6ebe2c75ef owned by bgruening (prior install required)
  - **package_lapack_3_4** revision a6b8f46acca7 owned by bgruening (prior install required)
  - **package_atlas_3_10** revision 25dc49b0d6d5 owned by bgruening (prior install required)
  - **package_openbabel_2_3** revision 3a933ff17df5 owned by bgruening (prior install required)
  - **package_scipy_0_12** revision e4f395310680 owned by bgruening (prior install required)
  - **package_lapack_3_4** revision a6b8f46acca7 owned by bgruening (prior install required)
  - **package_atlas_3_10** revision 25dc49b0d6d5 owned by bgruening (prior install required)
  - **package_numpy_1_7** revision ad6ebe2c75ef owned by bgruening (prior install required)
  - **opsin** revision 12640f433fd7 owned by bgruening
  - **molecule_datatypes** revision a1474892287e owned by bgruening
  - **rdkit** revision 0ab075fb42f9 owned by bgruening
  - **package_rdkit_2012_12** revision 5b30ea84ba25 owned by bgruening (prior install required)
ChemicalToolBox Dependency Graph
A demonstration using the Galaxy API

install_tool_shed_repositories.py
   --api 22be3b2e392a64
   -l http://localhost:8763
   --url http://localhost:9009/
   --name chemicaltoolbox
       -o bgruning
       -r 1018e3cee313
       --tool-deps
   --repository-deps
   --panel-section-name 'Chemical Tool BoX'
Acknowledgments

Special thanks to:

- Björn Grüning, author of the chemicaltoolbox repository – [http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox](http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox)

- Dave Bouvier
The Galaxy Team

http://wiki.galaxyproject.org/GalaxyTeam
Acknowledgments

- The Galaxy Team
  [http://wiki.galaxyproject.org/GalaxyTeam](http://wiki.galaxyproject.org/GalaxyTeam)
- The Galaxy Community – thousands of users and contributors
- Funding sources
  - NSF–ABI
  - NIH–NHGRI
  - Beckman Foundation
  - Huck Institutes at Penn State
  - Pennsylvania Department of Public Health
  - Emory University