Workflows for Computer Aided Drug Discovery: New Twitter for the Old Problem

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Abstract:

Computer-aided drug discovery (CADD) is becoming more accessible with the availability of personal supercomputers, especially given the recent advancement in GPU computing. The cloud computing infrastructure represented by Amazon EC2 offer an attractive solution for those who only require intermittent access to computing resources on demand. However, workflow management for the complexity in the CADD process and the ease of use for biomedical students and researchers remain a challenging problem. A large number of workflow tools exist, yet the applications remain isolated in supercomputer centers, or clusters. New applications are increasing rapidly and require better and easier ways to be available for biomedical researchers.

We have continued to use the Avian Flu Grid infrastructure to study inhibitor development for influenza pandemics. The associated research and development effort from NBCR, PRAGMA projects explore the deployment of scientific applications as services, and the use of workflow tools such as Vision, Kepler, Nimrod/K and Vistrails to support the service mashups often required to support the CADD process. The central toolkit that provides a Web Service based simple protocol for these different workflow clients is the Opal toolkit, an open source software available at sourceforge.net. Our effort has resulted in a prototype CADD workflow software based upon Vision, but the underlying services are accessible from a number of other clients.

The availability of these scientific application services advances the cyberinfrastructure for biomedical research, and generates more requirements for focused, user friendly scientific research and collaboration environment, including ways to build and/or leverage the social networks like Facebook, Twitter, LinkedIn and Google Wave for scientists.