MURPA 2009 Seminar Program: Next Seminar Thursday 23 April 10-11am

Integration of machine learning approaches in avian flu drug discovery workflows

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Venue: Seminar Room 135, Building 26 Clayton

Abstract:

Biomedical, translational and clinical research through increasingly complex computational modeling and simulation generate enormous potential for personalized medicine and therapy, and an insatiable demand for advanced cyberinfrastructure (CI). New programming models and workflow management tools are required to allow researchers to move quickly from pilot studies to large-scale simulation experiments. Massive datacenters, aka, cloud computing, have emerged to offer very large petascale computing environment. Effective middleware that help existing scientific applications to gain integrated access to computation, data and visualization resources are required. They must be highly reusable and yet customizable based upon the specific needs of a particular scientific community, such as computer aided drug discovery (CADD).

The Avian Flu Grid (AFG) virtual organization (VO) is dedicated to collaborative research on antiviral drug discovery for potentially pandemic influenza viruses. Using the software as a service (Saas) paradigm, we have established services for required applications in the computer aided drug discovery pipeline, including the molecular dynamics applications such as NAMD and virtual screening applications such as AutoDock. These services may be invoked within the usual user environment such as ADT (AutoDockTools) or advanced workflow management tools such as Vision, Kepler, Nimrod/K, while the jobs are executed remotely on grid or cloud resources such as the PRAGMA grid, TeraGrid or Amazon EC2.

In earlier studies, we have identified novel inhibitors for H5N1 neuraminidase N1 in ensemble based virtual screening experiments using the relaxed complex method. We have recently focused on the integration of machine learning applications in computer aided drug discovery workflows, aka, cheminformatics workflows, with the participation of MURPA students. We have evaluated the application of 1-, 2- or 3-Dimensional molecular descriptors or fingerprints in the classification, expansion, and optimization of these N1 inhibitors. Integration of these machine learning algorithms and appropriate visualization technology for multidimensional datasets into CADD pipelines will expedite the development of effective therapies against infectious diseases. These cross-disciplinary studies present exciting translational research opportunities, and pose interesting challenges for efficient CI development.

Bio

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