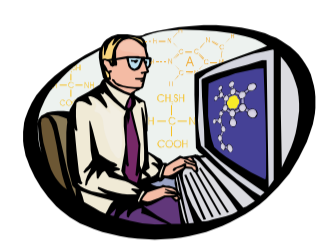


Hung-Chun Lee, Pei-Ying Yao, Yu-Hsuan Chen, Hsin-Yen Chen, Chon-Chen Lee, Li-Yung Ho, Ying-Ta Wu, Simon C. Lin  
Grid Computing Center, Academia Sinica, Genomic Research Center, Academia Sinica

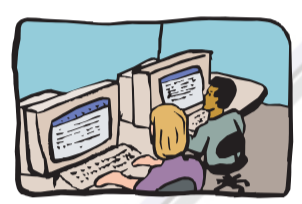
The first avian flu data challenge and the WISDOM project have demonstrated that the grid is an ideal environment providing “on-demand” resources for large-scale docking simulations of drug analysis. The objective of the project is to deliver a productive system enabling biologists to run the docking simulations and to manage the docking results on the grid as simple as using a desktop utility in the daily research.

#### Opening up the grid from the end-users' desktop

- Portable client APIs ready to be integrated with desktop applications
- As of today, the system has been used by biologists to run docking simulations on the grid

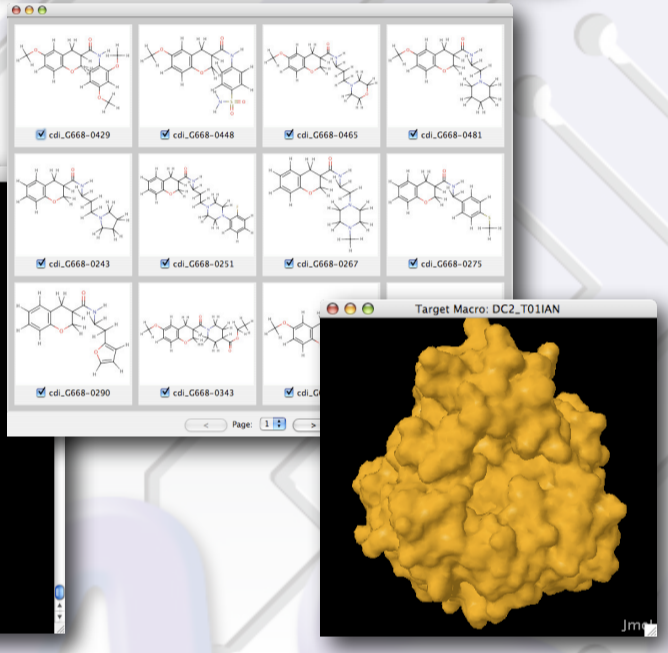


> login();

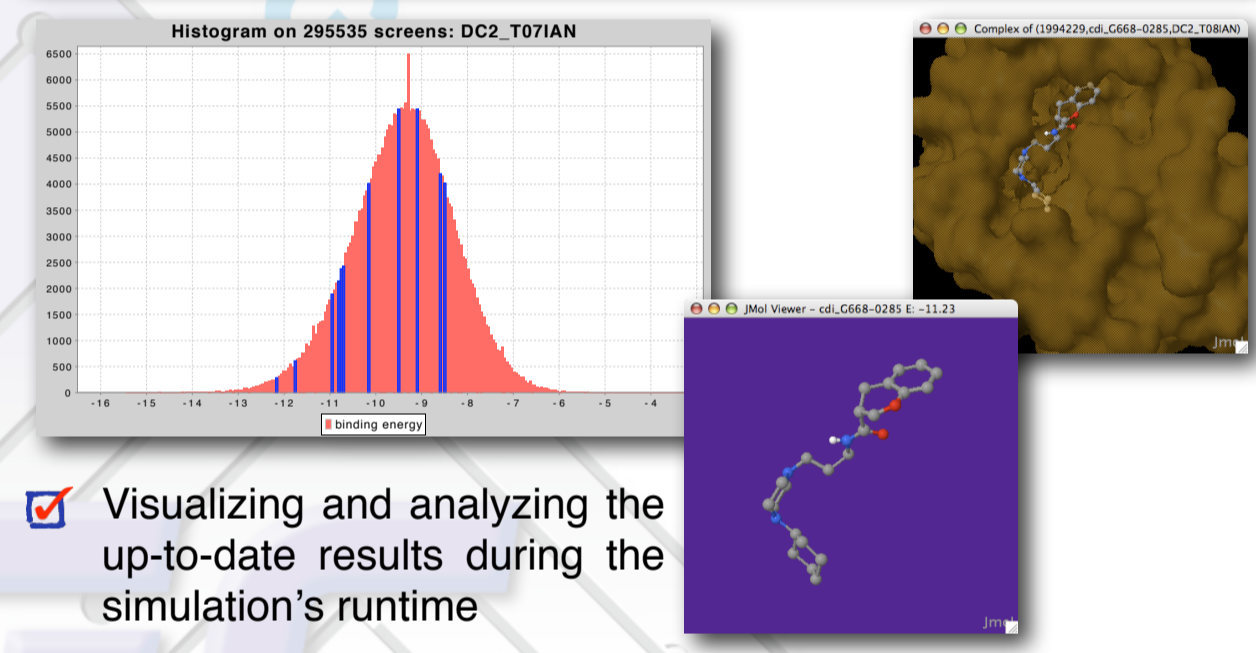


#### Intuitive interface for launching simulations

- Preparing simulation jobs in an application-oriented way

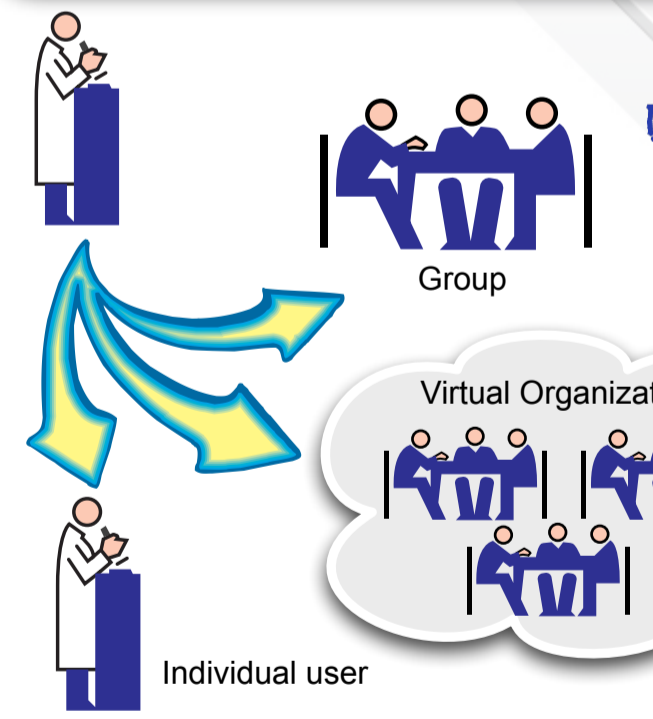


#### Online visualization & data analysis



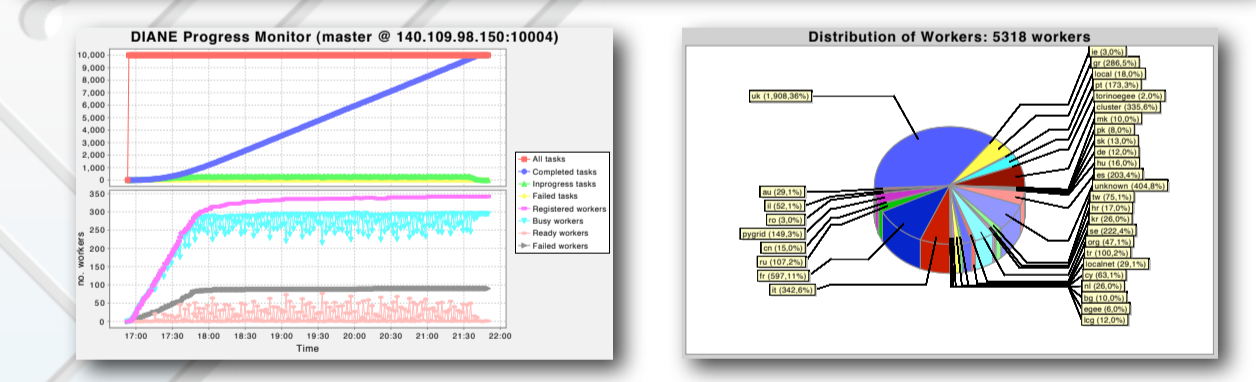
- Visualizing and analyzing the up-to-date results during the simulation's runtime

#### Team work & collaborations



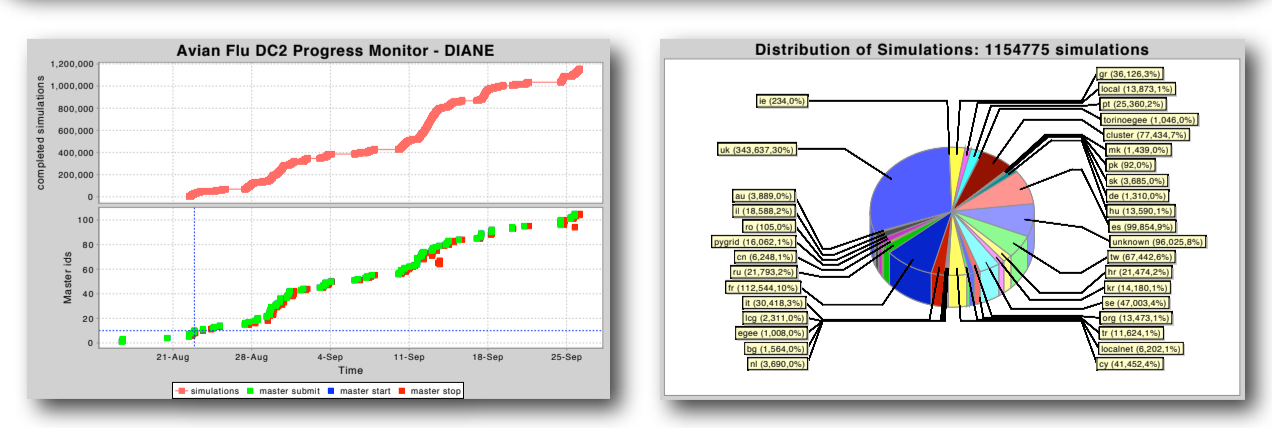
- Sharing simulation jobs and results with an individual user, a group of users or a Virtual Organization

#### Reliability & scalability



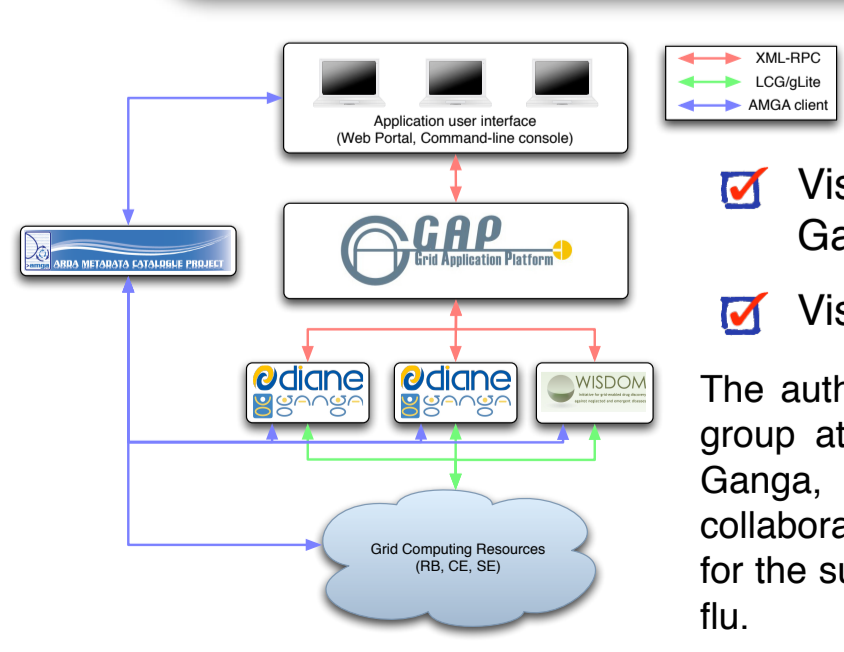
- Adopting grid technologies to support large-scale production
- Exposing end users to a stable and reliable simulation environment on the dynamic grid environment

#### Second H5N1 avian flu drug analysis



- Pre-screening phase: 2007.08.23 - 2007.09.23
- Simulations on the grid are generated by biology users
- ~ 1.2 M simulations (22 CPU years) completed in 1 month

#### Architecture & core technology



- Visit another on-line demo of Ganga / DIANE (#178)
- Visit AMGA poster (#177)

The authors would like to thank to the ARDA group at CERN for the technical support on Ganga, DIANE and AMGA; the WISDOM collaborators and the grid resource providers for the support on the grid challenges on avian flu.