UPDATES ON GRID COMPUTING APPLICATIONS IN ATENEO DE MANILA UNIVERSITY

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Current Grid Applications

- As part of the EUAsiaGrid Project
  http://www.euasiagrid.org
- 1.0 In Silico Screening for Anti-Dengue Drug Discovery Using the Grid Application Platform (GAP) (Biomedical Application)
- 2.0 Landslides and Floods Disaster Mitigation: Data Warehousing, Risk Assessment, Monitoring, Modelling and Simulation (Disaster Mitigation Application)
- 3.0 Economic Modeling (Evolutionary Trade) and Poverty Alleviation (Social Science Application)
Biomedical Application

- Title: In Silico Screening for Anti-Dengue Drug Discovery Using the Grid Application Platform (GAP)
Status and Future Work

- An interdisciplinary group of researchers in the School of Science and Engineering of Ateneo de Manila University is conducting a search for a shortlist of ligands with some of the lowest energies that can be tested for wet laboratory techniques through the following procedures:
  - Nucleotide sequences are downloaded from NCBI.
  - These are aligned and the conserved regions are noted.
  - The consensus sequence is taken.
  - It is transcribed and translated to its amino acid sequence.
  - The three-dimensional structure of this sequence is then computed, subjected to wet laboratory techniques.
Status and Future Work

- To validate the structure, homology techniques are done to confirm changes in structure.
- If there is no significant change, the active sites are assumed to be conserved.
- This PDBQS file of this protein is prepared in silico.
- Ligands libraries with analogue structures to the substrate are taken.
- Apart from small molecules, short peptides and nucleotide chains are seen as possible candidates.
- The ligand files are prepared.
- These are docked into the protein PDBQS file via GAP (Grid Application Platform).
- A shortlist of candidate ligands with some of the lowest energies is produced by the end of this study.
- These ligands and protein target can be fabricated and subjected to wet laboratory techniques.
Status and Future Work

- The research is on-going.

- At least 10 researchers from AdMU have applied for and issued Grid Certificates by the ASGC and have become members of the EUAsiaGrid VO. It requires the use of GAP (Grid Application Platform).

- The AdMU EUAsiaGrid staff has developed a training manual specific for the dengue fever application.

- Since AdMU has no wet lab capability, it will need outside collaborators, such as the Academia Sinica Grid Computing Center (Taiwan) and HealthGrid (France) – both EUAsiaGrid Partners --, to assist in identifying specific targets from the shortlisted candidate ligands.

- Once the specific targets have been identified through wet laboratory techniques, the team from AdMU will again use GAP for the docking procedure.
Disaster Mitigation/Climate Change Application

- Landslides and Floods Disaster Mitigation: Data Warehousing, Risk Assessment, Monitoring, Modelling and Simulation
Landslides and Floods/Climate Change Application

- A research team from the School of Science and Engineering of AdMU is collaborating with scientists at the Manila Observatory (MO) for Landslides and Floods Disaster Mitigation.
- The goal is to establish a grid-based database of Philippine geographical data related to landslides and floods that can be analyzed and visualized through the EUAsiaGrid infrastructure.
- Cellular automata/Agent based model of landslides and floods are being developed and will be used for the simulations.
Evolutionary Trade Modeling and Poverty Alleviation

- Figure: World Poverty Map Based on Landscan Data

Figure 2. Poverty index calculated by dividing the LandScan 2004 population count by the average digital number of the DMSP satellite F15 nighttime lights from 2003.
Evolutionary Trade Modeling and Poverty Alleviation

- Figure: Human Poverty Map
- (Source: http://www.worldmapper.org/display.php?selected=174)
(3) Evolutionary Trade Modeling and Poverty Alleviation
Evolutionary Trade Modeling and Poverty Alleviation

- A team from AdMU is collaborating with economists from the Asian Development Bank (ADB) for evolutionary trade modeling in the East South Asia Region, which is one of the poorest regions in the world (East India, Bangladesh, Bhutan and Nepal).

- The goal of the study is to determine the impact of investments in the economic growth of the region using a geographic information system, cellular automata/agent based modeling technique, and the grid infrastructure.
Evolutionary Trade Modeling and Poverty Alleviation

- Currently, the mathematical and computational aspects of the evolutionary trade model is being assessed.

- An international start-up workshop was held in October 2009 at the Asian Development Bank (which includes representatives from EUAsiaGrid partners AdMU and ASGC) to assess and refine the trade model, the grid computing platform to be used and the computing resource requirements for the complex economic modeling in the East South Asia Region.

- A tie-up with the EUIndiaGrid may be helpful.

- In the future, the techniques and experiences gained from this study may be applied to the Philippines and the rest of Southeast Asia using the EUAsiaGrid infrastructure.
THANK YOU.

- For comments, inquiries and feedback, please contact:

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