

Grid workflow tools for performing molecular computations

Elisa Abate

Monash University

Melbourne, Australia

15 July, 2009



The Proposed Research

- Using grid and workflow tools (Nimrod/K & Kepler) available here at Monash University, we will manage the molecular computations of computational chemistry software (APBS & GAMESS) used by Prof. Baldrige's group.
- By streamlining the workflow, we can carry out ligand-protein parametric experiments that investigate changes in structure, environment, and methodology.

Recent Progress

- Two more workflows have been received from Tirath and each is more complicated than the previous (for reference: Wkflw #1 < #2 < #3 in complicity).
 - Wkflw #1 has been run successfully
 - Wkflw #2 is undergoing troubleshooting
 - Current version of GAMESS may not be compatible
 - Wkflw #3 has yet to be tested

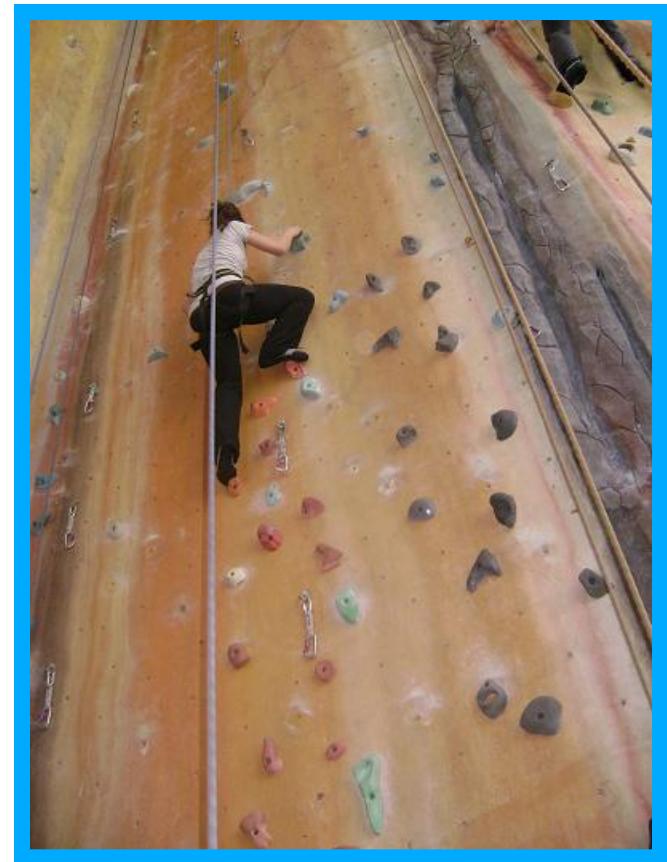
Recent Progress (cont)

- APBS-0.3.2 has been installed locally
 - The latest version (1.2.0) was not installed so that there would be consistency between Zurich's and Monash's equipment.
 - Initial issues have recently been solved and examples have been run successfully.

Next Week

- Hopefully, all troubleshooting issues will be solved
- Focus will turn towards the incorporation of APBS into the workflow (Wkflw #3)
- Assignment from Tirath: Create an actor within Kepler that takes a .pqr file input and produces a .acc file output
 - The actor is then to be compared to his “answer key”

Australia!



Australia!

