

Grid workflow tools for performing molecular computations

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The Progress To Date

- Nimrod tutorial completed for explanation of Nimrod/E, /O, /OI, /G, and /K
- Established connections on my personal laptop to remote Linux machine
 - Consequently, I can now run Nimrod/K
- Successful installation of GAMESS on server
- Successful installation of OpenBabel on server

Progress To Date (cont)

- Successful execution of GAMESS examples
 - Not before solving a whole slew of programming issues... Special thanks to Colin!
- Multiple attempts to run Tirath's sample workflow with Nimrod
 - Multiple errors were encountered and resolved, but there are still more to be ironed out... More thanks to Colin!

Next Week

- Receive more complicated workflows from Tirath
 - Study, understand, and execute the workflows
- Further study how to create GAMESS input files
- Study the chemistry theory that is the basis of GAMESS
 - Specifically, the theory behind individual commands and functions

Australia!



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