Pfound – Detailed Progress Report

Progress report on *Pfound-VMD* system during my visit to Northern Ireland – Coleraine, 24 Out.-28 Nov. 2006

Work plan proposed on July 2006:

- improve pfoundBasic package
- write a manual concerning pfoundBasic package usage
- optimize calculation of SASA
- produce pictures/movies of the protein/trajectory being deposited
- distribution of jobs to multiple nodes on behemoth

FYI:

In order to keep track of file location, I'll use the following nomenclature through out this text:

- pfound related files are on $pfound (say, pfound=/data/moldyn/pfound)

Detailed work progress accomplished:

- **Pfound pack version**
  - pfound_11dez06.tgz

- **User pfound on behemoth**
  - a new user named pfound was created on behemoth
  - Pfound-VMD will from now on be implementated under $pfound **[still in tests]**
  - this will allow better control of all cron jobs related to the project, as well as avoids conflicts with file permissions
  - presently, only members of group moldyn have rwx privileges to pfound user space

- **VMD and the Pfound system – data organization**
  - re-organization of directories on $pfound dir
  - a set of molecular dynamics sample data produced by different MD softwares was added to $pfound/data for testing purposes **[tested only NAMD data]**
  - taken care of directory permissions allowing the DW to communicate with VMD [w privileges]

- **Updated pfoundBasic package**
  - cleaning and polishing of package
  - current working version 1.0
  - package location: $pfound/lib

- **Scheduling behemoth jobs through crontab daemon**
  - wrote cron.readme file to explain how to edit pfound user crontable

- wrote cron.entries file as an example to tweak user crontable
- vmd now loads a startup file (vmd.rc) where some of the VMD stage/display properties are defined (display size, background color, protein default representation and all associated rep values, ...)
- cron.* files location: $pfound/scripts

- **Main batch job called by crontab – pfound.cron**
  - cleaning, polishing and optimization of pfound.cron
  - a more detailed survey of how pfound.cron works was written (see file header)
  - file location: $pfound/scripts

- **2D graphics of relevant property data**
  - optimization of ascii file headers (property files, eg. *.rmsd, *.rmsf ...), to be fed to *Grace* program (*gracebat*)
  - added P-found tags, timestamps and simulation ID info to each ascii file
  - added angstrom symbol to relevant axis labels (hexadecimal to ASCII char conversion)
  - other 2D formating issues

- **Generating movies and pictures**
  - all procedures dealing with multimedia files were implemented on a new package (::pfoundMultimedia::), based on vmdmovie1.5 plugin
  - wrote procedure to generate an animated gif (rotation) from the first frame of the deposited trajectory as well as a animated gif trajectory movie (::pfoundMultimedia::genMovie::)
  - wrote procedures to generate a trajectory movie in mpeg format (::pfoundMultimedia::genMovie::)
  - wrote procedure to save a protein data bank (pdb) file from the first frame of the deposited trajectory (::pfoundMultimedia::writePdb); in the near future, this pdb will allow the browser (trough a plugin like Jmol), to display a 3D representation of the protein.
  - package location: $pfound/lib

- **VMD and Pfound system – manual**
  - a manual is being written, explaining how VMD interacts with pfound DW, as well as a short explanation of all relevant procedures needed during a trajectory processing.
  - file location: $pfound/docs/TechReport_vmd_packages.odt

- **Started but not finished/tested**
  - implementation of a new package (orient1.01) based on orient1.0 ; this package will allow to orient the molecule (1st frame) so that its three principal axes are aligned with the *x*, *y*, and *z* directions
  - ray trace the videos/snapshots with PovRay

2Do stuff:

- read trajectories not by its file extension, but using the more complex "mol load" facilities provided by VMD

- implement procedures to deal with periodic boundary problems on the uploaded trajectories to the DW (wrapp on, wrapp off, whole protein molecules, ...)
- work on the display of 2D matrices using xmgr/grace nomenclature, producing .png files; already have some ascii file examples of how to to this.
- distribution of jobs to multiple nodes on behemoth (Scyld/Clustermatic slave node)
- optimize the calculation of Solvent Accessible Surface Areas (SASA); compare the performance/results/algorithm with the VMD built-in command "measure sasa"
- Implement on pfound webpage, a plugin to visualize in 3D the structure of the deposited protein, as well as to see relevant movies (multiple pdb models on the same file). The implementation of this type of plugins should be done by the admin of the webpage.
- Test with GROMACS and AMBER trajectories
- Since the calculation of molecular properties rely heavily on 3rd party software, I should write a proc in order to test if all the required software is correctly installed. Currently the external software list is: naccess, NetPBM, ImageMagick, Grace
- Adding a Progress Bar for the Elapsed Time to trajectory movies

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