FittingWizard : plans for further improvements

Florent Hédin, Prashant Gupta

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1 LJ parameters fitting

The goal would be to extend the current application in order to have the possibility to use it for performing a fit of the Lennard-Jones parameters for the CHARMM forcefield.

The easiest way of doing that would be to add a button on the last panel of the current software, i.e. when the ESP fit is done. Then a new panel would appear for setting up parameters for the LJ fit.

2 Roadmap

Here is a first estimate of the required steps:

- Choose the type of properties used for estimating the LJ parameters: density, heat of vaporisation, ...
- Generate CHARMM compatible coordinates (COR or PDB) and topology (PSF).
- Atom types: may be give to the user the opportunity to edit the atom types manually before generating the COR and PSF files.
- Initial guess for the well depth and distance parameters, and increment used: also define a lower and upper limit for the possible values ?
- Generate the corresponding input files for CHARMM.
- Copy files to distant server, similarly to what was done with Gaussian.
- Run CHARMM on the distant server.
- Either: (i) copy back output files on the local machine and run the scripts locally, or (ii) run those scripts on the distant server and just copy back final results to the local machine. Will depend on the computational cost required by those scripts.

3 Technical considerations

3.1 Coordinates and topology files

The current software uses XYZ coordinates, not read by CHARMM, and containing no topology or connectivity information.

Then it is necessary to generate a COR or PDB file, and a topology PSF file. We currently have a script from V. Zoete for building a PSF, and need to check for some scripts written by group members for generating COR or PDB.

An alternative would be to have look at the possibility offered by **OpenBabel**. (http://openbabel.org/wiki/Babel).

3.2 CHARMM input files

We need to have a proper template that will be used for preparing the input files. Ideally the user would be able to run the fitting without having to modify this template, but giving this opportunity to the user would be useful.