

User guide for the DPG Energetics library

Installation

1. First, use the makefile in the DPG directory to build the DPG library
 2. Then, use the Makefile in the DPGB directory to build the energetics computation program.
- Additional note for the parallel version
 - Download and install cilk++
 - Set the path to the cilk directory inside the Makefiles
 - Carry out the steps 1-2 mentioned above.

Usage with TexMol

Execute-

TestFastGB “.pqr File” “.quad File” “outputFile”

- Note about the inputs
 - One can use PDB2PQR to generate the .pqr file from a .pdb file
 - .quad files can be generated using either the MolSurf or the TexMol package
- Output is a text file containing
 - The born radii of the atoms
- Also prints the following on the standard output
 - Time taken to compute the Born radii using DPG
 - Time taken to compute the Born radii naively
 - Average error the born radii
 - Gpol computed with Born radii computed using DPG
 - Gpol computed with Born radii computed naively

Overview of the software

