Calculating surface electrostatic potential on a pre-computed van der Waal's (vdw) sphere of a single charged atom

How to run:

Check that you have all the input files: Nval.pdb, born.siz, born.crg, Nval_vdw.pdb

To run it, type:

<path>/delphi param_vdw_single_atom.prm > vdw_sa.log

Press enter key, and you should get the results.

Output files: Nval_vdw.pot

*Note: <path> is the full path where the delphi executable file is located.

Details of the run:

This example is used to calculate the electrostatic potential on the van der Waal's surface of a single charged atom (Nitrogen, vdw radius: 1.82 Angstrom). The pre-computed van der Waal's surface (**Figure 1**) is fed to the program as a PDB file (Nval_vdw.pdb) using the frc input option.

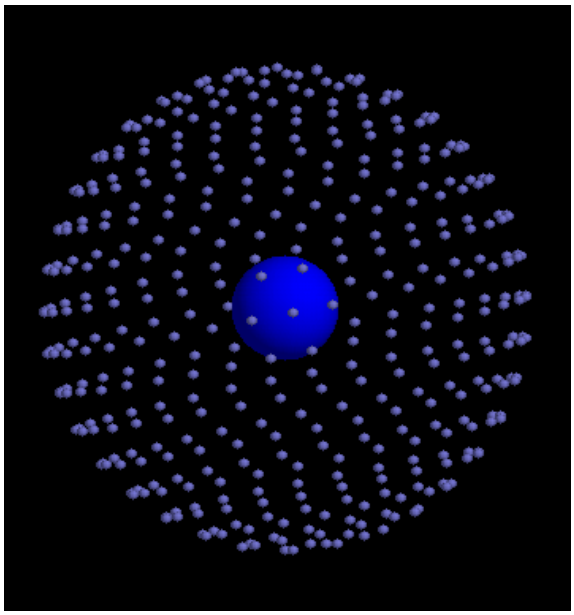

Figure 1. The van der Waal's surface (a collection of dot surface points colored in magenta) of an N atom. The large blue sphere at the center represents the atomic position.

The outfile is written in 'Nval_vdw.pot' which lists the surface potentials (as in the last column) against the dot surface points (x,y,z).

ATOM DESCRIPTOR			ATOM COORDINATES (X,Y,Z)			GRID PT.
N	VAL	10	0.0000	0.0000	1.8200	66.7764
N	VAL	10	0.1670	0.2640	1.7930	64.3238
N	VAL	10	-0.1330	0.2830	1.7930	65.0925
N	VAL	10	-0.3100	0.0390	1.7930	65.8366
N	VAL	10	-0.1990	-0.2400	1.7930	66.1831
N	VAL	10	0.0960	-0.2970	1.7930	65.5393
N	VAL	10	0.3020	-0.0780	1.7930	65.0955
N	VAL	10	0.5370	0.3000	1.7130	62.8861
N	VAL	10	0.3220	0.5240	1.7130	62.9421
N	VAL	10	0.0250	0.6150	1.7130	63.3701
…	…	…				

We also provide a program (in Fortran) and instructions to generate the van der sphere of your choice – which is to be found at: generate_vdw_sphere_single_atom/

Follow the instructions in the README text file in the same folder.

This vdw surface generation code is part of the software distribution named the Complementarity Plot (https://en.wikipedia.org/wiki/Complementarity_plot) resulting from the following paper.

Basu, S.; Bhattacharyya, D.; Banerjee, R. Self-Complementarity within Proteins: Bridging the Gap between Binding and Folding. Biophys. J. 2012, 102 (11), 2605–2614.