This directory contains several example use cases of popular electrostatics modeling software DelPhi. Before running any of the examples discussed below, first we shall set the DelPhi executable file in the DELPHI_EXE environment variable, for this purpose a bash script `set-delphi-path.sh` is provided in the directory. Execute this bash script as:

```
bash  set-delphi-path.sh
```

This script is required to be run only once, after running this script close your terminal and open it again, now environment variable `DELPHI_EXE` must be available. One can check it by running command:

```
echo $DELPHI_EXE
```

Above command should print the absolute path of the DelPhi executable present in the directory.

In addition some examples require `python3` for running multiple DelPhi times to obtain discussed quantities. Following `python3` packages are also needed to run these cases successfully. These examples are as follows, these packages can be installed on machines with internet connection running latest releases of Linux distributions like Ubuntu 18.04 or later as:

```
pip3 install numpy scipy matplotlib pandas
```

The examples provided are as follows.

Using DelPhi for computing solvation energy

Example_3.1.1: This directory contains two sub directories Ex1 and Ex2, which provide example cases of computing solvation energy of two cases: a. solvation of a charged sphere, and b. solvation of a protein-protein complex (here discusses barnase-barstar complex). All the necessary input files are also provided.

Using DelPhi for computing saltation energy:

Example_3.1.2: This directory also contains two sub directories Ex1 and Ex2, which provide example cases of computing solvation energy of two cases: a. saltation energy of a charged sphere, and b. saltation energy of a protein-protein complex (here discusses barnase-barstar complex). The analytical

solution of charged sphere case is also known thus DelPhi results are compared with analytical result. All the necessary input files are also provided.

Using DelPhi for Computing electrostatic potential on a surface (Zeta potential)

Example_3.1.3: This directory contains an example to demonstrate computing electrostatic potential on a surface of lysozyme.

Using DelPhi for Computing electrostatic potential, energy of interaction and forces between two sets of atoms

Example_3.1.4: In this example we demonstrate using DelPhi for computing force via frc module. In this example we compute electrostatic force on a particle due to a system of two charged particles.

Using focusing module of DelPhi

Example_3.1.5: The example calculates potential and electric field generated by barnase and onto a particular residue Asp39 of its partner barstar.

Using DelPhi for computing Electrostatic component of binding energy

Example_3.1.6: In this case we demonstrate both approaches (traditional 2-dielectric and Gaussian model) for computing electrostatic component of binding energy. In this example we use barnase-barstar complex for demonstration.

Using DelPhi for computing Salt dependence of binding energy using traditional 2-dielectric model

Example_3.1.7: In this example we demonstrate how to use DelPhi for computing salt dependence of binding energy using traditional 2-dielectric approach taking barnase-barstar complex.

Using DelPhi for computing Salt dependence of binding energy using Gaussian model

Example_3.1.7: In this example we demonstrate how to use DelPhi for computing salt dependence of binding energy using traditional gaussian model approach taking barnase-barstar complex.