**Example of working with FRC file**

This example shows how we can use “frc” option.

Consider three atoms as shown in Figure 1.

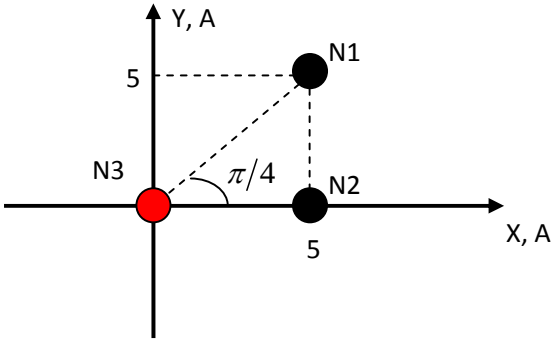


Figure 1.

Suppose that atom N1 has positive charge $Q_1 = 10 \cdot e$ and N2 has positive charge $Q_2 = 20 \cdot e$. And we want to know what potential in red point (0,0) is. And what components of electrical field in this point are.

For our goal we should use the following pdb-file, which is made of the two atoms, N1 and N2 (“my.pdb”):

```
ATOM   1    N1  GLN D  10      5.0    5.0    0.0
ATOM   2    N2  GLN D  10      5.0    0.0    0.0
```

The potential and the components of the electrostatic field will be collected the red point (Fig. 1) with coordinates are provided in “my1.pdb”:

```
ATOM   1    N3  GLN D  10      0.0    0.0    0.0
```

The corresponding crg- and siz- files look like usual (note that N3 atom is not provided in “crg” file to avoid the contribution of N3 on itself):

“my.crg”

```
N1   GLN     10.000
N2   GLN     20.000
```

“my.siz”

```
N1   GLN   1.0
N2   GLN   1.0
```

In param-file we need to use the command “site(argument)”, specifically in this case site(a,f,p). This command makes DelPhi to reports the potentials and electrostatic field components at the positions of the subset of atoms specified in the frc file. The atoms specified in frc file should not be charged in the delphi run.

Param-file “param.txt”

```
gsize=161
scale=2.0
in(pdb,file="my.pdb")
in(frc,file="my1.pdb")
in(siz,file="my.siz")
in(crg,file="my.crg")
indi=2.0
exdi=80.0
prbrad=1.4
salt=0.00
bndcon=2
maxc=0.0001
linit=800
site(a,f,p)
out(frc,file="my.frc")
energy(s,c,g)
```

Output file “my.frc” contains necessary lines with information regarding potential and components of electrical field:

```
ATOM DESCRIPTOR      GRID PT.    GRID FIELDS: (Ex, Ey, Ez)
N3   GLN D 10        38.1317   -6.7208   -1.0031    0.0000
```

Let’s check with analytical results:

$$\varphi = \frac{1}{4 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_{ext}} \cdot \left( \frac{Q_1}{d_1} + \frac{Q_2}{d_2} \right) \tag{1}$$

Also we need to convert the energy in eq. (1) in DelPhi units, namely [kT/e]. Having in mind that $k = 1.38 \cdot 10^{-23} \mathrm{JK}^{-1}$ is the Boltzmann constant, and $T = 297.33\mathrm{K}$ is absolute temperature, $e \approx 1.6 \cdot 10^{-19}\mathrm{C}$ is the elementary charge, $\varepsilon_{\mathrm{int}} = 80$ is interior dielectric constant eq. (1) gives:

$$\varphi = \frac{1}{4 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_{ext}} \cdot \left( \frac{Q_1}{d_1} + \frac{Q_2}{d_2} \right) \cdot \frac{e}{k \cdot T} = 38.035, \frac{k \cdot T}{e} \tag{2}$$

For X-component of electrical fields:

$$E_x = -\frac{1}{4 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_{ext}} \cdot \left( \frac{Q_1}{d_1^2} \cdot \cos\left( \frac{\pi}{4} \right) + \frac{Q_2}{d_2^2} \right) \cdot \frac{e \cdot A}{k \cdot T} = -6.613, \frac{k \cdot T}{e \cdot A} \tag{3}$$

And for Y-component of electrical fields:

$$E_y = -\frac{1}{4 \cdot \pi \cdot \varepsilon_0 \cdot \varepsilon_{ext}} \cdot \frac{Q_1}{d_1^2} \cdot \sin\left( \frac{\pi}{4} \right) \cdot \frac{e \cdot A}{k \cdot T} = -0.993, \frac{k \cdot T}{e \cdot A} \tag{4}$$

Where $A = 10^{-10}$ means angstroms.

For example the relative error for potential is

$$\varepsilon = \left| \frac{\varphi - \varphi^{DelPhi}}{\varphi} \right| \approx 10^{-3}. \tag{5}$$

Note that analytical expressions are obtained for point charge, while in the Delphi example, we deal with distributed charges over the grid. This is the reason for slight discrepancies.