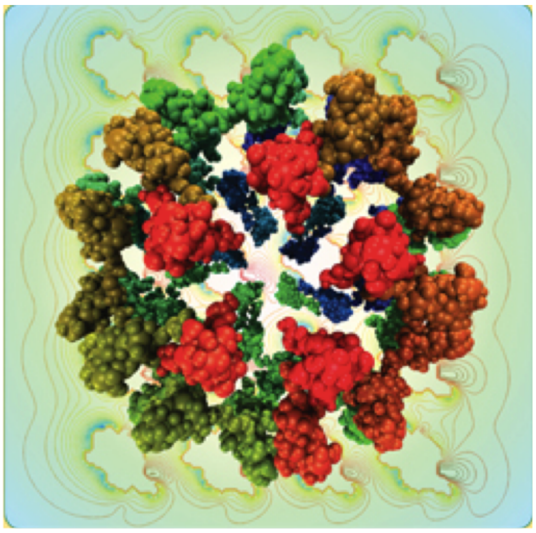
# Reference Manual
Poisson Boltzmann Analytical Model (PB-AM)



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For more information, please visit http://thglab.berkeley.edu

**Cover Illustration:** An exploded view of a Brome Mosaic Virus capsid composed of T = 1 particles (PDB: 1YC6), represented as collections of overlapping spheres, is shown. PB-SAM is a new semi-analytical approach to efficiently solve the linearized Poisson-Boltzmann equation using multipole formalisms for overlapping spheres. The background shows the potential profile for an array of 601YC6 monomers computed using this method.

**Recommended Citations:**

When citing PB-AM in the literature, the following citation should be used
I. Lotan and T. Head-Gordon (2006). An analytical electrostatic model for salt screened interactions between multiple proteins J. Chem. Theory Comput 2, 541-555.

When citing PB-SAM in the literature, the following citations should be used
1. E.-H. Yap and T. Head-Gordon (2010). New and efficient Poisson-Boltzmann solver for interaction of multiple proteins J. Chem. Theory Comput. (Journal cover) 6, 2214-2224.
2. E.-H. Yap and T. Head-Gordon (2013). Calculating the bimolecular rate of protein?protein association with interacting crowders. J. Chem. Theory Comput. 9(5), 2481-2489.
3. O. N. Demerdash, E.-H. Yap and T. Head-Gordon (2014). Advanced potential energy surfaces for condensed phase simulation. Ann. Rev. Phys. Chem. 65, 149-174.

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# Table of Contents

# Chapter 1

# Introduction

The Poisson-Boltzmann Analytical and Semi-Analytical models solve the linearized Poisson-Boltzmann Equation (PBE) for systems hitherto not possible using traditional PBE solvers. This manual describes the methods and their associated suite of programs. We will refer to each method by their acronyms: PB-AM and PB-SAM. There is much shared capability between the two softwares, so when an application or usage can be applied to both, we will refer to both of them as PB-[S]AM, with the S in square brackets. The PBE software suite is licensed as a collection of freely available program under a GPL license.

## 1.1 PB-AM

The first general analytical solution for computing the screened electrostatic interaction between large numbers of macromolecules of arbitrarily complex charge distributions, assuming they are well described by spherical low dielectric cavities in a higher dielectric medium in the presence of a Debye-Hückel treatment of salt. The method exploits multipole expansion theory for the screened Coulomb potential such that it can describe direct charge-charge interactions and all higher-order cavity polarization effects between low dielectric spherical cavities containing their charges, while treating these higher order terms correctly at all separation distances. The analytical solution is general to arbitrary numbers of macromolecules, is efficient to compute, provides for the first time the ability to provide new benchmarks for other numerical solutions to the linearized Poisson-Boltzmann equation. A number of utilities are described below that use PB-AM results.

## 1.2 PB-SAM

A semi-analytical extension of the PB-AM method. It too is capable of computing the interactions of multiple molecules with complex charge distributions, but because of its semi-analytical approach, molecules are now represented as a collection of overlapping spheres. This allows for a more complex description of the molecule in comparison to the analytical method. The applications below also apply to the semi-analytical method.

## 1.3 Physical Calculations

The PB-[S]AM results allow for fast calculation of physically important quantities. Specifically this program can calculate the interaction energy of, and the force and torque applied to each molecule. These results may be written into a file or printed to the terminal.

## 1.4 Brownian Dynamics

This package also implements dynamics simulations using the Brownian protocol developed by Ermak and McCammon[1]. At each time step, the translation and rotation due to the applied force and torque, respectively, are calculated and added to random components of motion. The user can specify spatial and temporal termination conditions for the simulation and write the trajectory to specified files.

## 1.5 Electrostatics

Another possible output of PB-AM, the user can specify a configuration of an arbitrary number of molecules and get a 2-dimensional or 3 dimensional potential landscape of the system. We have provided example plotting tools, and the 3-dimensional output may be uploaded in VMD for visualization.

[1]Ermak, D. L.; McCammon, J. A. *J. Chem. Phys.* 1978, *69*, 1352–1360.

# Chapter 2

# The Poisson-Boltzmann Analytical Method

## 2.1 PB-AM formulation

PB-AM is an analytical solution to the linearized Poisson-Boltzmann equations for multiple spherical objects of arbitrary charge distribution in an ionic solution. The linearized Poisson-Boltzmann equation is given as:

$$\nabla[\epsilon(r)\nabla\phi(r)] - \epsilon(r)\kappa^2\phi(r) = 4\pi\rho(r)$$

$$\phi_{out}^{(i)} = \phi_{out}^{(i)}\Big|_{r=a_i}$$

$$\epsilon_s \frac{\partial \phi_{out}^{(i)}}{\partial r} = \epsilon_s \frac{\partial \phi_{out}^{(i)}}{\partial r}\Big|_{r=a_i}$$

Exploiting fast-multipole methods, this boundary value problem can be reduced to the following system of linear equations.

$$A = \Gamma \cdot (\Delta \cdot T \cdot A + E)$$

A(i) represents the effective multipole expansion of the charge distributions of molecule (i). E(i) is the free charge distribution of molecule (i). $\Gamma$ is a dielectric boundary-crossing operator, $\Delta$ a cavity polarization operator, T an operator that transforms the multipole expansion to a local coordinate frame. More details on the method are available in Lotan, Head-Gordon (2006).

### 2.1.1 Physical Calculations

From the above formulation, computation of the interaction energies ($\Omega^{(i)}$) is given as follows:

$$\Omega^{(i)} = \frac{1}{\epsilon_s}\left\langle \sum_{j\neq i}^{N} T \cdot A^{(j)}, A^{(i)} \right\rangle$$

Where $\langle M, N \rangle$ denotes the inner product. When energy is computed, forces follow as:

$$\mathbf{F}^{(i)} = \nabla_i \Omega^{(i)} = \frac{1}{\epsilon_s}[\langle \nabla_i T \cdot A^{(i)}, A^{(i)} \rangle + \langle T \cdot A^{(i)}, \nabla_i A^{(i)} \rangle]$$

The method to calculate the torque $\boldsymbol{\tau}^{(i)}$ on molecule is outside the scope of this manual, but is discussed extensively in Lotan, Head-Gordon (2006).

### 2.1.2 Brownian Dynamics

Brownian dynamics simulations are implemented by treating each molecule as a Brownian particle experiencing a conservative force $\mathbf{F}^{(i)}$ and torque $\boldsymbol{\tau}^{(i)}$, as well as friction and random force due to the solvent. The translation $\Delta r_i$ and rotation $\Delta\theta_i$ for a time step $\Delta t$ are then given by

$$\Delta r^{(i)} = \frac{D_{i,trans}\Delta t}{k_B T}\mathbf{F}^{(i)} + \mathbf{S}_i(\Delta t)$$
$$\Delta\theta^{(i)} = \frac{D_{i,rot}\Delta t}{k_B T}\boldsymbol{\tau}^{(i)} + \boldsymbol{\Theta}_i(\Delta t)$$

where $D_{i,trans}$ and $D_{i,rot}$ are the translation and rotational diffusion coefficients for molecule $i$, respectively and $\mathbf{S}_i(\Delta t)$ and $\boldsymbol{\Theta}_i(\Delta t)$ are the stochastic components of translation and rotation, respectively, which have the following properties:

$$\langle \mathbf{S}_i \rangle = 0, \qquad \langle \mathbf{S}_i^2 \rangle = 2D_{i,trans}\Delta t$$
$$\langle \boldsymbol{\Theta}_i \rangle = 0, \qquad \langle \boldsymbol{\Theta}_i^2 \rangle = 2D_{i,rot}\Delta t$$

### 2.1.3 Electrostatics

In a similar manner to the interaction energy calculations in the Physical Calculations section, the electrostatics computes the potential at any point in space exterior to the molecules, $\mathbf{r}$, as the inner product of all the solved effective multipole expansions $A^{(j)}$ with a local multipole expansion of a single positive charge at position, $\mathbf{r}$.

$$\Phi_{out}(\mathbf{r}) = \frac{1}{\epsilon_s}\left\langle \sum_{j=1}^{N} T \cdot A^{(j)},\, A(\mathbf{r}) \right\rangle$$

## 2.2 Use

### 2.2.1 Installation

To install this program, first download the source code from the GitHub repository:

```
$ git clone https://github.com/davas301/pb_solvers.git clone_dir
```

Then navigate to the cloned directory `clone_dir`. From here, make a `build` directory, use CMake to create a make file and then make the program. This is done as follows:

```
$ cd clone_dir
$ mkdir build
$ cd build
$ cmake ..
$ make pbam
```

An executable named `pbam` will now be in `clone_dir/build/bin`.

## 2.3 Input Information

**Input Files**

The program executable requires an input file as a command line parameter. The input file contains the various arguments and parameters that one may wish to set when running the program. Each line of the input file contains a keyword followed by a variable number of whitespace-delimited parameters, e.g.:

```
keyword1    param1    param2
keyword2    param1    param2    param3
```

Each keyword is described in the table below, along with its associated parameters.

| Keyword | Parameters | Description |
|---|---|---|
| runname | <name> | <name> is desired internal name of this run. |
| attypes | <numtypes> | Set the number of different atom types to <numtypes>. |
| pqr | <idx> <fpath> | The molecule index for this xyz file. Provide input PQR file at <fpath>. |
| xyz | <idx> <fpath> | The molecule index for this xyz file. Provide input XYZ file at <fpath>. |
| transrot | <idx> <fpath> | The molecule type index for this translation/rotation file that can be input instead of a xyz file. Provide input file at <fpath>. |
| randorient | | If you want your molecules to be randomly rotated, use this flag |
| units | <units> | Set the units of output to <units>. The current options are: `jmol` (Joules/mole), `kT` (kT/e) and `kcalmol` (kCal/mole). |
| salt | <con> | Set salt concentration in the system to <con>. |
| temp | <T> | Set system temperature to <T> |
| idiel | <ival> | Set the interior dielectric constant to <ival>. |
| sdiel | <sval> | Set the solvent dielectric constant to <sval>. |
| pbc | <boxlength> | Set size of periodic box to <boxlength>. |
| random | <seed> | Seed the internal random number generator with <seed>. |
| type | <idx> <ct> <movetype> <dtr> <drot> | Set attributes of an atom type, where <idx> is the integer id of this type, which can be 1 to <numtypes> (above). <ct> is the number of atoms of this type in the system and <movetype> describes the way this type is allowed to move in a dynamics run (`move`, `rot`, or `stat`). If <movetype> is `move`, then a translational diffusion coefficient <dtr> and a rotational diffusional coefficient <drot> are required. If <movetype> is `rot` then just <drot> is required. |

| **Keyword** | **Parameters** | **Description** |
|---|---|---|
| runtype electrostatics | <`gridpts`> | Will run electrostatics calculations. <`gridpts`> is an optional integer describing the number of evenly spaced points in each dimension to perform calculations on. |
| dx | <`fname`> | For electrostatics. Will write the results of electrostatics calculations for every 3D grid point to <`fname`>, in the same output format as APBS dx file. |
| 3dmap | <`fname`> | For electrostatics. Will write the results of electrostatics calculations for points on the surface of the molecules in the system. |
| gridct | <`ct`> | For electrostatics. <`ct`> is the number of 2D grids to output. |
| grid2d | <`idx`> <`fname`> <`axis`> <`val`> | For electrostatics. Set attributes of a grid output where <`idx`> is the integer id of this grid, which can be 1 to <`ct`> (above). Will write output of calculations for a cross section along <`axis`> (`x`, `y`, or `z`) at <`value`>. |

| Keyword | Parameters | Description |
|---|---|---|
| runtype dynamics | `<outname>` `<ntraj>` | Will perform a brownian dynamics run. A directory where trajectory information will be stored in and the number of trajectories is required. |
| termct | `<ct>` | Set number of termination conditions to `<ct>`. |
| termcombine | `<andor>` | Set how termination conditions will be combined. `<andor>` should be `and` or `or`. Default is `or`. |
| term | `<idx>` `<type>` `<val>` `<mols>` | Set attributes of a termination condition where `<idx>` is the integer id of this condition, which can be 1 to `<ct>` (above). `<type>` can be `time`, `x<=`, `y<=`, `z<=`, or `r<=` (or the `>=` equivalents of these), `<val>` is the value where the simulation will terminate and `<mols>` is a whitespace-delimited list of molecular indices that this condition applies to (`time` requires 0, and all else require 1). |
| term `<idx>` contact | `<confile>` `<pad>` | Set attributes of contact termination condition, where `<idx>` is the integer id of this condition, `<confile>` is a path to a file containing the contact information, and `<pad>` specifies a correction for the case when the contact distance cannot be reached due to the spherical assumption of the model. See below for more info. |
| xyz | `<idx>` `<trajidx>` `<fpath>` | `<idx>` is the molecule index for this xyz file. Provide input XYZ file at `<fpath>`. For the dynamics run, a starting configuration is needed for each trajectory for all the molecule types, so there should be `<ntraj>` xyz lines for each molecule, the trajectory number denoted by `<trajidx>`. |
| runtype energyforce | `<outfilename>` | Will calculate the interaction energy, the forces and torques for the system input. `<outfilename>` is a filename that you would like the information printed to. If none is entered, the information will be printed to the command line. |

### 2.3.1 System inputs: PQR, XYZ, Translation/Rotation and Contact files

#### PQR File

All the options above require a **PQR** file name. A PQR file can be generated from a PDB file using the PDB2PQR program, available as a web server or for download at:

http://nbcr-222.ucsd.edu/pdb2pqr_1.9.0/
http://www.poissonboltzmann.org/docs/pdb2pqr-installation/

It may also be formatted manually. The general format of a PQR file is as follows, and is whitespace-delimited:

```
recName serial atName resName chainID resNum X Y Z charge rad
```

| Parameter | Description |
|---|---|
| `recName` | A string that should either be ATOM or HETATM. |
| `serial` | An integer that provides the atom index |
| `atName` | A string that provides the atom name. |
| `resName` | A string that provides the residue name. |
| `chainID` | An optional string that provides the chain ID of the atom. |
| `residueNumber` | An integer that provides the residue index. |
| `X Y Z` | Three floats that provide the atomic coordinates. |
| `charge` | A float that provides the atomic charge (in electrons). |
| `Rad` | A float that provides the atomic radius (in Å). |

#### XYZ File

The **XYZ** file simply specifies the desired molecule centers for a given molecule type.

```
mol1X mol1Y mol1Z
mol2X mol2Y mol2Z
mol3X mol3Y mol3Z
```

#### Translation/Rotation File

**Translation/Rotation** Instead of a XYZ file, one can input a file specifying the translations and rotations that should be applied to each molecule of a particular type. For these files, we follow the PDB standard for rotation matrices and translation vectors, which is as follows:

```
mol1 rot_1_11 rot_1_12 rot_1_13 trans_1_1
mol1 rot_1_21 rot_1_22 rot_1_23 trans_1_2
mol1 rot_1_31 rot_1_32 rot_1_33 trans_1_3
mol2 rot_2_11 rot_2_12 rot_2_13 trans_2_1
mol2 rot_2_21 rot_2_22 rot_2_23 trans_2_2
mol2 rot_2_31 rot_2_32 rot_2_33 trans_2_3
```

where `mol1` and `mol2` are indices of the molecule of the type this file applies to, `rot_i_jk` is the `j,k` index of the rotation matrix for molecule `i` and `trans_i_j` is the `j`th element in the translation vector for molecule `i`.

### Contact File

**Contact** files describe contacts between two molecular types. Generally this information is used to determine if a dynamics simulation should be terminated (e.g. terminate a simulation after two proteins have docked). The contact file contains lines with the format:

```
moltype1 at1 moltype2 at2 dist
```

where `moltype1` and `moltype2` are indices of the molecular types, `at1` is the index of an atom from the first molecular type, `at2` is the index of an atom from the second molecular type and `dist` is the maximum distance between the two atoms that defines the contact. Note that sometimes these distances cannot be reached due to the assumption in this model that the molecule is spherical. To correct for this case, one must specify a ”pad” distance that is defined as the maximum distance between the radial projections of the atoms onto the surface of their respective spheres that defines a contact.

## 2.4 Example files and outputs

### 2.4.1 Physical calculations

#### Example physical calculations runfile

name: `run.energyforce.inp`:

```
runtype energyforce
runname energyforce.2sp.jmol.out

units jmol
salt 0.01
temp 353
idiel 4
sdiel 78

attypes 1
type 1 2
pqr 1 single_charge.pqr
xyz 1 positions_2.xyz
```

The files for PQR and XYZ are:
name: `single_charge.pqr`:

```
ATOM      1  N    NTR     0       1.000     0.000     0.000  -1.0000  3.7300
ATOM      1  N    NTR     0       0.000     1.000     0.000  -1.0000  6.3200
```

name: `positions_2.xyz`:

```
-10.0   23.4   -8.7
  0.0    0.0   -2.5
```

To run:

```
$$ ../../bin/pbam run.energyforce.inp
```

And the resulting file:
name: `energyforce.2sp.jmol.out`:

```
My units are Joules/Mol
MOLECULE #1
        POSITION: [-10, 23.4, -8.7]
        ENERGY: 1328.86
        FORCE: 1.19858e+08, [-36.6012 1.19858e+08 -1.65408e-05]
        TORQUE: 1.78426e+06, [1.28425 1.78426e+06 1.9978e-06]
MOLECULE #2
        POSITION: [0, 0, -2.5]
        ENERGY: 1328.86
        FORCE: 1.19858e+08, [36.6012 -1.19858e+08 1.65408e-05]
        TORQUE: 1.78354e+06, [1.28372 1.78354e+06 1.99699e-06]
```

### 2.4.2 Brownian Dynamics

#### Example dynamics runfile

name: `run.dynamics.inp`:

```
runtype dynamics 2
runname dyn_cont_barn
```

```

salt 0.01
temp 298
idiel 4
sdiel 78

termct 1
termcombine or
term 1 contact 2.5 1 2

attypes 2
type 1 2 move 0.015 0.000045
pqr 1 1BRS_chainA.pqr
xyz 1 1 pos_1_1.xyz
xyz 1 2 pos_1_2.xyz

type 2 2 move 0.015 0.000045
pqr 2 1BRS_chainD.pqr
xyz 2 1 pos_2_1.xyz
xyz 2 2 pos_2_2.xyz
```

The files for PQR (first 5 lines) and XYZ files for the first trajectories are:
name: `1BRS_chainA.pqr`:

```
ATOM   1700  N    ALA B   1       20.757  52.394  30.692     0.1414   1.8240
ATOM   1702  CA   ALA B   1       20.602  52.680  29.268     0.0962   1.9080
ATOM   1703  C    ALA B   1       19.286  52.138  28.675     0.6163   1.9080
ATOM   1704  O    ALA B   1       18.578  51.351  29.318    -0.5722   1.6612
ATOM   1705  CB   ALA B   1       21.739  52.033  28.476    -0.0597   1.9080
```

name: `pos_1_1.xyz`:

```
61.25 61.25 61.25
-26.25 61.25 -26.25
```

name: `1BRS_chainD.pqr`:

```
ATOM      1  N    LYS D   1       48.330  40.393   9.798     0.0966   1.8240
ATOM      2  CA   LYS D   1       47.401  39.287   9.370    -0.0015   1.9080
ATOM      3  C    LYS D   1       47.507  38.911   7.890     0.7214   1.9080
ATOM      4  O    LYS D   1       47.126  39.582   6.905    -0.6013   1.6612
ATOM      5  CB   LYS D   1       45.995  39.632   9.817     0.0212   1.9080
```

name: `pos_2_1.xyz`:

```
-26.25 61.25 61.25
61.25 -26.25 61.25
```

To run:

```
$$ ../../bin/pbam run.dynamics.inp
```

And the resulting files:
name: `dyn_cont_barn_[traj#].xyz`: VMD readable XYZ file that shows the trajectory of molecules in the system. The time that is snapshot was printed from is given on the same line as the word Atom. The atoms of your input file are currently labeled N, and the coarse-grain center is labeled "X" in the first column of the XYZ file.

```
3135
Atoms. Timestep (ps): 0
N    -7.241     -0.530     18.703
N    -6.015     -0.503     17.910
```

```
N    -5.784     0.840    17.188
N    -6.682     1.690    17.128
N    -6.066    -1.580    16.827
N    -7.519    -1.481    18.863
N    -7.084    -0.079    19.584
```

name: `dyn_cont_barn_[traj#].dat`: Statistics from simulation printed out at the same time as each XYZ snapshot. The energy is not computed and should be ignored.

```
My units are Internal. Time (ps) 500.4
MOLECULE #1
   POSITION: [0, 0, 0]
   ENERGY: 0
   FORCE: 3.39124e-06, [1.69863e-06 2.07547e-06 6.5356e-07]
   TORQUE: 2.55224e-05, [-2.11728e-05 1.00774e-05 3.08631e-05]
MOLECULE #2
   POSITION: [87.211, 43.861, 21.691]
   ENERGY: 0
   FORCE: 3.65373e-06, [-1.87502e-06 -2.21744e-06 -7.27314e-07]
   TORQUE: 1.91656e-05, [8.14396e-06 -1.22678e-05 1.56284e-05]
```

name: `dyn_nam_barn.stat` : Details about how each simulation has terminated and the time at which this occurred.

```
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 1.32367e+06
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 1.15712e+06
System has fulfilled condition: Type 0 and Type 1 are within  2.50;  at time (ps)
    1.90603e+06
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 2.18533e+06
System has fulfilled condition: Type 0 and Type 1 are within  2.50;  at time (ps)
    1.59066e+06
```

### 2.4.3 Electrostatics

#### Example electrostatics runfile

name: `run.electrostatic.inp`:

```
runtype electrostatics 140
runname electrostatic

units kT
salt 0.01
temp 298
idiel 4
sdiel 78

dx out.dx

3dmap electro_map.out

gridct 2
grid2D 1 out.x.0.dat x 0
grid2D 2 out.x.-1.dat x -1

attypes 2
type 1 2
pqr 1 single_charge.pqr
xyz 1 positions_2.xyz

type 2 2
pqr 2 pos_charge.pqr
```

```
xyz 2 positions_pos.xyz
```

The files for PQR and XYZ files are:

name: `single_charge.pqr`:

```
ATOM    1  N   NTR    0      0.000   1.000   0.000   4.0000  0.3200
ATOM    1  N   NTR    0      0.000   0.000  -1.000   4.0000  0.3200
ATOM    1  X   CEN    0      0.000   0.000   0.000   0.0000  2.0000
```

name: `positions_2.xyz`:

```
  0.0   0.0   -5.0
  0.0   0.0    5.0
```

name: `pos_charge.pqr`:

```
ATOM    1  N   NTR    0      0.000   1.000   0.000  -4.0000  0.3200
ATOM    1  N   NTR    0      0.000   0.000  -1.000  -4.0000  0.3200
ATOM    1  X   CEN    0      0.000   0.000   0.000   0.0000  2.0000
```

name: `positions_pos.xyz`:

```
  0.0   5.0   0.0
  0.0  -5.0   0.0
```

To run:

```
$$ ../../bin/pbam run.electrostatic.inp
```

And the resulting files:

name: `out.dx`:

```
# Data from PBAM Electrostat run
# My runname is out.dx and units kT/e
object 1 class gridpositions counts 140 140 140
origin -4 -9 -9
delta 0.0571429 0.0e+00 0.0e+00
delta 0.0e00 0.128571 0.0e+00
delta 0.0e00 0.0e+00 0.128571
object 2 class gridconnections counts 140 140 140
object 3 class array type double rank 0 items 2744000 data follows
2.7203115e-01  3.0271755e-01  3.3459723e-01
3.6769040e-01  4.0201595e-01  4.3759129e-01
.....
-1.3185519e-01  -1.5849252e-01  -1.8359631e-01
-2.0722087e-01  -2.2942006e-01  -2.5024714e-01
-2.6975467e-01  -2.8799442e-01
attribute "dep" string "positions"
object "regular positions regular connections" class field
component "positions" value 1
component "connections" value 2
component "data" value 3
```

name: `electro_map.out`:

```
# Data from PBAM Electrostat run
# My runname is electro_map.out and units kT/e
grid 10 10 10
origin -4 -9 -9
delta 0.8 1.8 1.8
  0.00825   0.00006   -2.90002  -5.899956
  0.00822   0.00071   -2.90002  -5.902602
```

name: `out.x.0.dat`:

```
# Data from PBAM Electrostat run
# My runname is out.x.0.dat
units kT
grid 140 140
axis x 0
origin -9 -9
delta 0.128571 0.128571
maxmin 39.23 -39.23
    0.3605004      0.4030045      0.4474874      0.4940082      0.5426260      0.5933995
```

# Chapter 3

# The Poisson-Boltzmann Semi Analytical Method

## 3.1 PB-SAM formulation

PB-SAM builds on the PB-AM solution to the linearized Poisson-Boltzmann equation (LPBE). While PB-AM gives a general solution to the LPBE for an arbitrary number of spherical objects, the PB-SAM formulation extends that solution to arbitrary shape. Instead of representing a macromolecule (denoted as $I$) as a single sphere, each molecule is represented as a collection of overlapping spheres (with each sphere denoted as $k$).

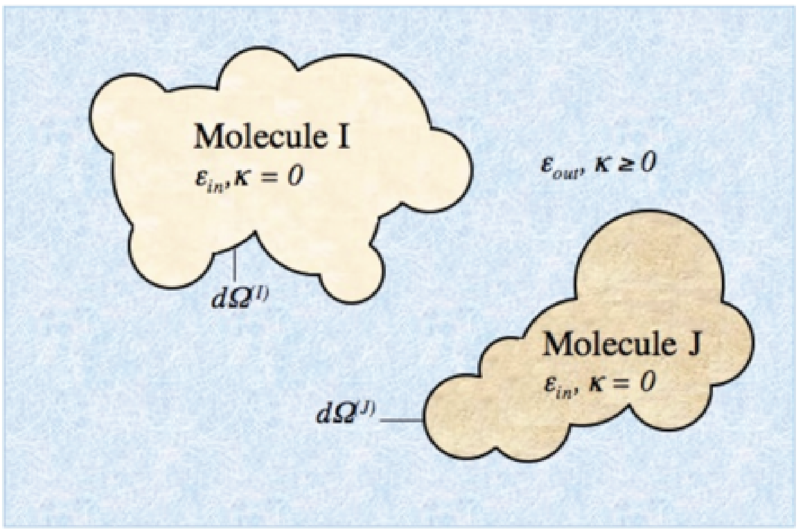

Molecule I
$\varepsilon_{in}, \kappa = 0$
$\varepsilon_{out}, \kappa \geq 0$
$d\Omega^{(I)}$
Molecule J
$\varepsilon_{in}, \kappa = 0$
$d\Omega^{(J)}$

Figure 3.1: Cartoon representation of PB-SAM.

Additional complexity is due to overlap between spheres. Whereas PB-AM has a single type of interaction (between separated spheres), PB-SAM has three types of interactions:

i. between spheres in different molecules
ii. between overlapping spheres within the same molecule
iii. between non-overlapping spheres within the same molecule

There is no dielectric discontinuity between spheres within the same macromolecule. More details on the method are available in Yap, Head-Gordon (2010).

### 3.1.1 Physical Calculations

The computation of the interaction energies ($\Omega^{(i)}$) remains essentially the same self-consistent equation as Eqn. 3.1

$$\Omega^{(i)} = \frac{1}{\epsilon_s} \sum_{k=1}^{N_S^{(I)}} \sum_{j=1, j\neq I}^{N} \sum_{l=1}^{N_S^{(j)}} \langle T \cdot H^{(j,l)}, H^{(i,k)} \rangle \tag{3.1}$$

However, now the interaction energy of a molecule $\Omega^{(i)}$ is the sum of the interaction energies of all its constituent spheres, and $H$ replaces $A$ Where $\langle M, N \rangle$ denotes the inner product. When energy is computed, forces follow as:

$$\mathbf{F}^{(i)} = \nabla_i \Omega^{(i)} = \frac{1}{\epsilon_s} [\langle \nabla_i T \cdot H^{(j,l)}, H^{(i)} \rangle + \langle T \cdot H^{(j,l)}, \nabla_i H^{(i)} \rangle]$$

The method to calculate the torque $\boldsymbol{\tau}^{(i)}$ on molecule is outside the scope of this manual, but is discussed extensively in Yap, Head-Gordon (2013).

### 3.1.2 Brownian Dynamics

Brownian dynamics simulations are implemented by treating each molecule as a Brownian particle experiencing a conservative force $\mathbf{F}^{(i)}$ and torque $\boldsymbol{\tau}^{(i)}$, as well as friction and random force due to the solvent. The translation $\Delta r_i$ and rotation $\Delta \theta_i$ for a time step $\Delta t$ are then given by

$$\Delta r^{(i)} = \frac{D_{i,trans} \Delta t}{k_B T} \mathbf{F}^{(i)} + \mathbf{S}_i(\Delta t)$$
$$\Delta \theta^{(i)} = \frac{D_{i,rot} \Delta t}{k_B T} \boldsymbol{\tau}^{(i)} + \boldsymbol{\Theta}_i(\Delta t)$$

where $D_{i,trans}$ and $D_{i,rot}$ are the translation and rotational diffusion coefficients for molecule $i$, respectively and $\mathbf{S}_i(\Delta t)$ and $\boldsymbol{\Theta}_i(\Delta t)$ are the stochastic components of translation and rotation, respectively, which have the following properties:

$$\langle \mathbf{S}_i \rangle = 0, \qquad \langle \mathbf{S}_i^2 \rangle = 2 D_{i,trans} \Delta t$$
$$\langle \boldsymbol{\Theta}_i \rangle = 0, \qquad \langle \boldsymbol{\Theta}_i^2 \rangle = 2 D_{i,rot} \Delta t$$

### 3.1.3 Electrostatics

In a similar manner to the interaction energy calculations in the Physical Calculations section, the electrostatics computes the potential at any point in space exterior to the molecules, $\mathbf{r}$, as the inner product of all the solved effective multipole expansions $H^{(j)}$ with a local multipole expansion of a single positive charge at position, $\mathbf{r}$.

$$\Phi_{out}(\mathbf{r}) = \frac{1}{\epsilon_s} \left\langle \sum_{j=1}^{N} T \cdot H^{(j)},\, H(\mathbf{r}) \right\rangle$$

## 3.2 Use

### 3.2.1 Installation

To install this program, first download the source code from the GitHub repository:

```
$ git clone https://github.com/davas301/pb_solvers.git clone_dir
```

Then navigate to the cloned directory `clone_dir`. From here, make a `build` directory, use CMake to create a make file and then make the program. This is done as follows:

```
$ cd clone_dir
$ mkdir build
$ cd build
$ cmake ..
$ make pbsam
```

An executable named `pbsam` will now be in `clone_dir/build/bin`.

## 3.3 Input Information

#### Input Files

The program executable requires an input file as a command line parameter. The input file contains the various arguments and parameters that one may wish to set when running the program. Each line of the input file contains a keyword followed by a variable number of whitespace-delimited parameters, e.g.:

```
keyword1    param1    param2
keyword2    param1    param2    param3
```

Each keyword is described in the table below, along with its associated parameters. They are pretty similar to the PB-AM inputs, but we repeat them here for PB-SAM inputs.

| **Keyword** | **Parameters** | **Description** |
|---|---|---|
| runname | `<name>` | `<name>` is desired internal name of this run. |
| attypes | `<numtypes>` | Set the number of different atom types to `<numtypes>`. |
| pqr | `<idx>` `<fpath>` | The molecule index for this xyz file. Provide input PQR file at `<fpath>`. |
| xyz | `<idx>` `<fpath>` | The molecule index for this xyz file. Provide input XYZ file at `<fpath>`. |
| surf | `<idx>` `<fpath>` | The molecule index for this vertex file. Provide input surface vertex file at `<fpath>`. |
| imat | `<idx>` `<fpath>` | The molecule index for this surface integral file. Provide input interaction matrix file prefix at `<fpath>`. There will be one for each CG sphere in the molecule. |
| exp | `<idx>` `<fpath>` | The molecule index for this vertex file. Provide expansion file prefix at `<fpath>`. There will be one for each CG sphere in the molecule, and are terminated by `sph[number].[H/F].exp`. |
| transrot | `<idx>` `<fpath>` | The molecule type index for this translation/rotation file that can be input instead of a xyz file. Provide input file at `<fpath>`. |
| randorient | | If you want your molecules to be randomly rotated, use this flag |
| units | `<units>` | Set the units of output to `<units>`. The current options are: `jmol` (Joules/mole), `kT` and `kcalmol` (kCal/mole). |
| tolsp | `<tolerance>` | Set coarse-graining tolerance in the system to `<tolerance>`. |
| salt | `<con>` | Set salt concentration in the system to `<con>`. |
| temp | `<T>` | Set system temperature to `<T>` |
| idiel | `<ival>` | Set the interior dielectric constant to `<ival>`. |
| sdiel | `<sval>` | Set the solvent dielectric constant to `<sval>`. |
| pbc | `<boxlength>` | Set size of periodic box to `<boxlength>`. |
| random | `<seed>` | Seed the internal random number generator with `<seed>`. |
| type | `<idx>` `<ct>` `<movetype>` `<dtr>` `<drot>` | Set attributes of an atom type, where `<idx>` is the integer id of this type, which can be 1 to `<numtypes>` (above). `<ct>` is the number of atoms of this type in the system and `<movetype>` describes the way this type is allowed to move in a dynamics run (`move`, `rot`, or `stat`). If `<movetype>` is `move`, then a translational diffusion coefficient `<dtr>` and a rotational diffusional coefficient `<drot>` are required. If `<movetype>` is `rot` then just `<drot>` is required. |

| **Keyword** | **Parameters** | **Description** |
|---|---|---|
| runtype electrostatics | <`gridpts`> | Will run electrostatics calculations. <`gridpts`> is an optional integer describing the number of evenly spaced points in each dimension to perform calculations on. |
| dx | <`fname`> | For electrostatics. Will write the results of electrostatics calculations for every 3D grid point to <`fname`>, in the same output format as APBS dx file. |
| 3dmap | <`fname`> | For electrostatics. Will write the results of electrostatics calculations for points on the surface of the molecules in the system. |
| gridct | <`ct`> | For electrostatics. <`ct`> is the number of 2D grids to output. |
| grid2d | <`idx`> <`fname`> <`axis`> <`val`> | For electrostatics. Set attributes of a grid output where <`idx`> is the integer id of this grid, which can be 1 to <`ct`> (above). Will write output of calculations for a cross section along <`axis`> (`x`, `y`, or `z`) at <`value`>. |

| Keyword | Parameters | Description |
|---|---|---|
| runtype dynamics | `<outname>` `<ntraj>` | Will perform a brownian dynamics run. A directory where trajectory information will be stored in and the number of trajectories is required. |
| termct | `<ct>` | Set number of termination conditions to `<ct>`. |
| termcombine | `<andor>` | Set how termination conditions will be combined. `<andor>` should be `and` or `or`. Default is `or`. |
| term | `<idx>` `<type>` `<val>` `<mols>` | Set attributes of a termination condition where `<idx>` is the integer id of this condition, which can be 1 to `<ct>` (above). `<type>` can be `time`, `x<=`, `y<=`, `z<=`, or `r<=` (or the `>=` equivalents of these), `<val>` is the value where the simulation will terminate and `<mols>` is a whitespace-delimited list of molecular indices that this condition applies to (`time` requires 0, and all else require 1). |
| term `<idx>` contact | `<confile>` `<pad>` | Set attributes of contact termination condition, where `<idx>` is the integer id of this condition, `<confile>` is a path to a file containing the contact information, and `<pad>` specifies a correction for the case when the contact distance cannot be reached due to the spherical assumption of the model. See below for more info. |
| xyz | `<idx>` `<trajidx>` `<fpath>` | `<idx>` is the molecule index for this xyz file. Provide input XYZ file at `<fpath>`. For the dynamics run, a starting configuration is needed for each trajectory for all the molecule types, so there should be `<ntraj>` xyz lines for each molecule, the trajectory number denoted by `<trajidx>`. |
| runtype energyforce | `<outfilename>` | Will calculate the interaction energy, the forces and torques for the system input. `<outfilename>` is a filename that you would like the information printed to. If none is entered, the information will be printed to the command line. |

### 3.3.1 System inputs: PQR, XYZ, Translation/Rotation, Contact and Vertex files

#### PQR file

All the options above require a **PQR** file name. A PQR file can be generated from a PDB file using the PDB2PQR program, available as a web server or for download at:

http://nbcr-222.ucsd.edu/pdb2pqr_1.9.0/
http://www.poissonboltzmann.org/docs/pdb2pqr-installation/

It may also be formatted manually. The general format of a PQR file is as follows, and is whitespace-delimited:

```
recName serial atName resName chainID resNum X Y Z charge rad
```

| Parameter | Description |
|---|---|
| `recName` | A string that should either be ATOM or HETATM. |
| `serial` | An integer that provides the atom index |
| `atName` | A string that provides the atom name. |
| `resName` | A string that provides the residue name. |
| `chainID` | An optional string that provides the chain ID of the atom. |
| `residueNumber` | An integer that provides the residue index. |
| `X Y Z` | Three floats that provide the atomic coordinates. |
| `charge` | A float that provides the atomic charge (in electrons). |
| `Rad` | A float that provides the atomic radius (in Å). |

#### XYZ file

The **XYZ** file simply specifies the desired molecule centers for a given molecule type.

```
mol1X mol1Y mol1Z
mol2X mol2Y mol2Z
mol3X mol3Y mol3Z
```

#### Translation/Rotation file

**Translation/Rotation** Instead of a XYZ file, one can input a file specifying the translations and rotations that should be applied to each molecule of a particular type. For these files, we follow the PDB standard for rotation matrices and translation vectors, which is as follows:

```
mol1 rot_1_11 rot_1_12 rot_1_13 trans_1_1
mol1 rot_1_21 rot_1_22 rot_1_23 trans_1_2
mol1 rot_1_31 rot_1_32 rot_1_33 trans_1_3
mol2 rot_2_11 rot_2_12 rot_2_13 trans_2_1
mol2 rot_2_21 rot_2_22 rot_2_23 trans_2_2
mol2 rot_2_31 rot_2_32 rot_2_33 trans_2_3
```

where `mol1` and `mol2` are indices of the molecule of the type this file applies to, `rot_i_jk` is the `j,k` index of the rotation matrix for molecule `i` and `trans_i_j` is the `j`th element in the translation vector for molecule `i`.

### Contact file

**Contact** files describe contacts between two molecular types. Generally this information is used to determine if a dynamics simulation should be terminated (e.g. terminate a simulation after two proteins have docked). The contact file contains lines with the format:

```
moltype1 at1 moltype2 at2 dist
```

where `moltype1` and `moltype2` are indices of the molecular types, `at1` is the index of an atom from the first molecular type, `at2` is the index of an atom from the second molecular type and `dist` is the maximum distance between the two atoms that defines the contact. Note that sometimes these distances cannot be reached due to the assumption in this model that the molecule is spherical. To correct for this case, one must specify a p̈add̈istance that is defined as the maximum distance between the radial projections of the atoms onto the surface of their respective spheres that defines a contact.

### Vertex file

The vertex file is given as follows:

```
 1669 95 3.00 1.50
2.965 12.871 -1.084 -0.751 -0.636 -0.175 0 81 2
3.241 11.952 -0.817 -0.936 -0.024 -0.353 0 69 2
3.026 11.791 -0.439 -0.792 0.084 -0.604 0 79 2
4.481 14.391 -3.026 -0.879 -0.246 -0.409 0 73 2
5.413 15.674 -0.948 -0.337 0.499 0.798 0 73 2
4.478 15.093 -0.297 0.286 0.886 0.365 0 81 2
4.930 15.004 -0.240 -0.015 0.945 0.326 0 71 2
4.072 13.663 0.763 -0.465 0.242 0.852 0 71 2
```

Where the first line is the number of vertex points, followed by information on the density of the surface, and the lines that follow indicate the cartesian locations of each vertex point, followed by the unit norm of the surface. This vertex file is used to coarse-grain the molecule.

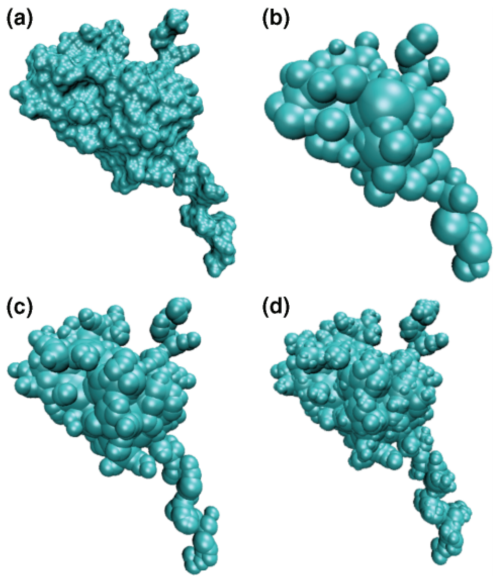


Figure 3.2: Representation of (a) solvent excluded surface generated by MSMS, (b) the CG surface with tolsp = $2\AA$, (c) CG surface with tolsp = $1\AA$, (d) CG surface with tolsp = $0.5\AA$.

## 3.4 Example files and outputs

### 3.4.1 Physical calculations

#### Example physical calculations runfile

name: `run.energyforce.inp`:

```
runtype energyforce
runname energyforce.2sp.jmol.out

units jmol
salt 0.01
temp 353
idiel 4
sdiel 78

attypes 1
type 1 2
pqr 1 single_charge.pqr
xyz 1 positions_2.xyz
```

The files for PQR and XYZ are:
name: `single_charge.pqr`:

```
ATOM      1  N   NTR    0      1.000   0.000   0.000  -1.0000  3.7300
ATOM      1  N   NTR    0      0.000   1.000   0.000  -1.0000  6.3200
```

name: `positions_2.xyz`:

```
-10.0  23.4  -8.7
  0.0   0.0  -2.5
```

To run:

```
$$ ../../bin/pbam run.energyforce.inp
```

And the resulting file:
name: `energyforce.2sp.jmol.out`:

```
My units are Joules/Mol
MOLECULE #1
        POSITION: [-10, 23.4, -8.7]
        ENERGY: 1328.86
        FORCE: 1.19858e+08, [-36.6012 1.19858e+08 -1.65408e-05]
        TORQUE: 1.78426e+06, [1.28425 1.78426e+06 1.9978e-06]
MOLECULE #2
        POSITION: [0, 0, -2.5]
        ENERGY: 1328.86
        FORCE: 1.19858e+08, [36.6012 -1.19858e+08 1.65408e-05]
        TORQUE: 1.78354e+06, [1.28372 1.78354e+06 1.99699e-06]
```

### 3.4.2 Brownian Dynamics

#### Example dynamics runfile

name: `run.dynamics.inp`:

```
runtype dynamics 2
runname dyn_cont_barn
```

```

salt 0.01
temp 298
idiel 4
sdiel 78

termct 1
termcombine or
term 1 contact 2.5 1 2

attypes 2
type 1 2 move 0.015 0.000045
pqr 1 1BRS_chainA.pqr
xyz 1 1 pos_1_1.xyz
xyz 1 2 pos_1_2.xyz

type 2 2 move 0.015 0.000045
pqr 2 1BRS_chainD.pqr
xyz 2 1 pos_2_1.xyz
xyz 2 2 pos_2_2.xyz
```

The files for PQR (first 5 lines) and XYZ files for the first trajectories are:
name: `1BRS_chainA.pqr`:

```
ATOM    1700   N    ALA B   1       20.757  52.394  30.692      0.1414   1.8240
ATOM    1702   CA   ALA B   1       20.602  52.680  29.268      0.0962   1.9080
ATOM    1703   C    ALA B   1       19.286  52.138  28.675      0.6163   1.9080
ATOM    1704   O    ALA B   1       18.578  51.351  29.318     -0.5722   1.6612
ATOM    1705   CB   ALA B   1       21.739  52.033  28.476     -0.0597   1.9080
```

name: `pos_1_1.xyz`:

```
61.25 61.25 61.25
-26.25 61.25 -26.25
```

name: `1BRS_chainD.pqr`:

```
ATOM       1   N    LYS D   1       48.330  40.393   9.798      0.0966   1.8240
ATOM       2   CA   LYS D   1       47.401  39.287   9.370     -0.0015   1.9080
ATOM       3   C    LYS D   1       47.507  38.911   7.890      0.7214   1.9080
ATOM       4   O    LYS D   1       47.126  39.582   6.905     -0.6013   1.6612
ATOM       5   CB   LYS D   1       45.995  39.632   9.817      0.0212   1.9080
```

name: `pos_2_1.xyz`:

```
-26.25 61.25 61.25
61.25 -26.25 61.25
```

To run:

```
$$ ../../bin/pbam run.dynamics.inp
```

And the resulting files:
name: `dyn_cont_barn_[traj#].xyz`: VMD readable XYZ file that shows the trajectory of molecules in the system. The time that is snapshot was printed from is given on the same line as the word Atom. The atoms of your input file are currently labeled N, and the coarse-grain center is labeled "X" in the first column of the XYZ file.

```
3135
Atoms. Timestep (ps): 0
N    -7.241    -0.530    18.703
N    -6.015    -0.503    17.910
```

```
N    -5.784    0.840    17.188
N    -6.682    1.690    17.128
N    -6.066   -1.580    16.827
N    -7.519   -1.481    18.863
N    -7.084   -0.079    19.584
```

name: dyn_cont_barn_[traj#].dat: Statistics from simulation printed out at the same time as each XYZ snapshot. The energy is not computed and should be ignored.

```
My units are Internal. Time (ps) 500.4
MOLECULE #1
  POSITION: [0, 0, 0]
  ENERGY: 0
  FORCE: 3.39124e-06, [1.69863e-06 2.07547e-06 6.5356e-07]
  TORQUE: 2.55224e-05, [-2.11728e-05 1.00774e-05 3.08631e-05]
MOLECULE #2
  POSITION: [87.211, 43.861, 21.691]
  ENERGY: 0
  FORCE: 3.65373e-06, [-1.87502e-06 -2.21744e-06 -7.27314e-07]
  TORQUE: 1.91656e-05, [8.14396e-06 -1.22678e-05 1.56284e-05]
```

name: dyn_nam_barn.stat : Details about how each simulation has terminated and the time at which this occurred.

```
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 1.32367e+06
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 1.15712e+06
System has fulfilled condition: Type 0 and Type 1 are within  2.50;  at time (ps)
    1.90603e+06
Molecule type 1 has fulfilled condition: r >= 500.00;  at time (ps) 2.18533e+06
System has fulfilled condition: Type 0 and Type 1 are within  2.50;  at time (ps)
    1.59066e+06
```

### 3.4.3 Electrostatics

#### Example electrostatics runfile

name: run.electrostatic.inp:

```
runtype electrostatics 140
runname electrostatic

units kT
salt 0.01
temp 298
idiel 4
sdiel 78

dx out.dx

3dmap electro_map.out

gridct 2
grid2D 1 out.x.0.dat x 0
grid2D 2 out.x.-1.dat x -1

attypes 2
type 1 2
pqr 1 single_charge.pqr
xyz 1 positions_2.xyz

type 2 2
pqr 2 pos_charge.pqr
```

```
xyz 2 positions_pos.xyz
```

The files for PQR and XYZ files are:

# Chapter 4

# Analysis Tools

## 4.1 Viewing PQR in VMD

Load pqr file

```
>> set selall [atomselect top "all"]
```

To center the pqr

```
>> $selall moveby {-x -y -z}
```

where x, y, and z are half the box length
Graphical representations: To view the charges inside the CG center, from the toolbar, select Graphics > Representations. In the selected atoms, type

```
not name X
```

Change the coloring method to Charge, and the Drawing Method to VDW. Then select the Create Rep button, and in the selected atoms, type

```
not name X
```

Change the Drawing Method to VDW and the Material to Transparent. The Graphical Representations and final images are in figure below.

## 4.2 Dynamics tools

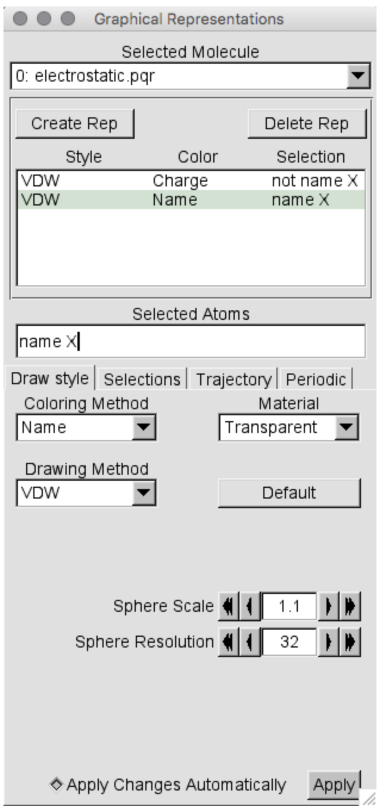
### 4.2.1 Viewing Dynamics in VMD

First load the PQR file, and then any XYZ files onto the same molecule.

## 4.3 Electrostatics tools

### 4.3.1 Viewing Electrostatics in VMD

To load electrostatic results: File > New Molecule. In the window that appears, toggle the *Load files for:* to select the currently loaded PQR file. Then select *Browse* to find the location of the dx file. Once found, hit the *Load* button and let the dx file load.



Selected Molecule
0: electrostatic.pqr

| Style | Color | Selection |
|---|---|---|
| VDW | Charge | not name X |
| VDW | Name | name X |

Selected Atoms
name X

Coloring Method: Name
Material: Transparent
Drawing Method: VDW
Sphere Scale: 1.1
Sphere Resolution: 32
◇ Apply Changes Automatically

Figure 4.1: Graphics

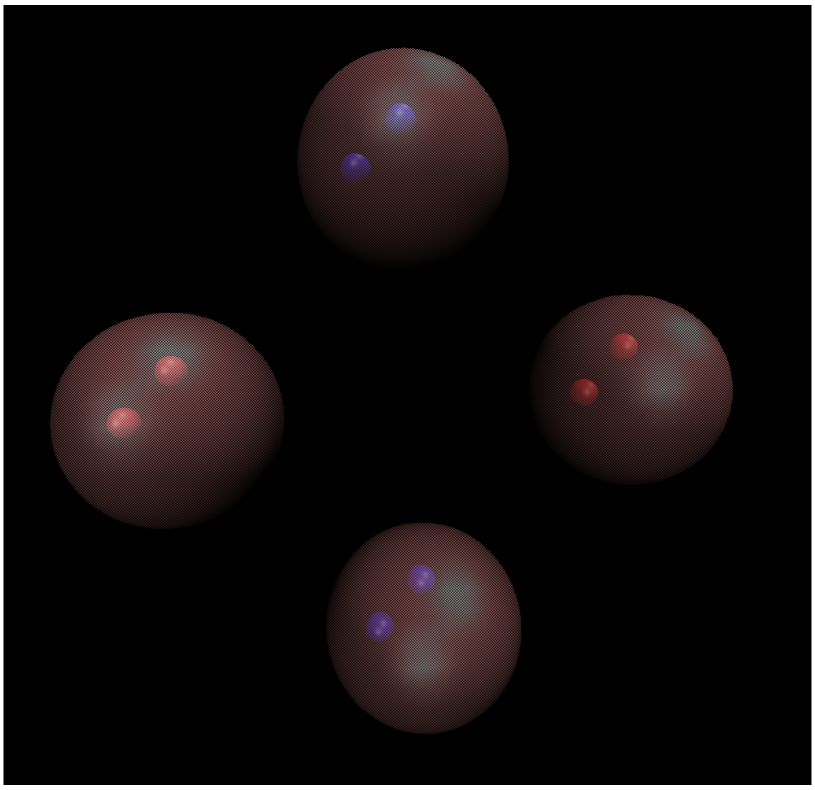
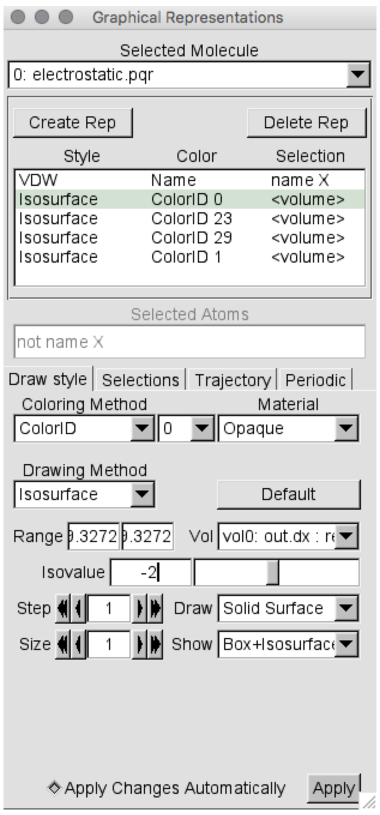


Figure 4.2: Final view



Selected Molecule
0: electrostatic.pqr

| Style | Color | Selection |
|---|---|---|
| VDW | Name | name X |
| Isosurface | ColorID 0 | <volume> |
| Isosurface | ColorID 23 | <volume> |
| Isosurface | ColorID 29 | <volume> |
| Isosurface | ColorID 1 | <volume> |

Selected Atoms
not name X

Coloring Method: ColorID 0
Material: Opaque
Drawing Method: Isosurface
Range ).3272 ).3272 Vol vol0: out.dx : r
Isovalue -2
Step 1 Draw Solid Surface
Size 1 Show Box+Isosurfac
◇ Apply Changes Automatically

Figure 4.3: DX Graphics

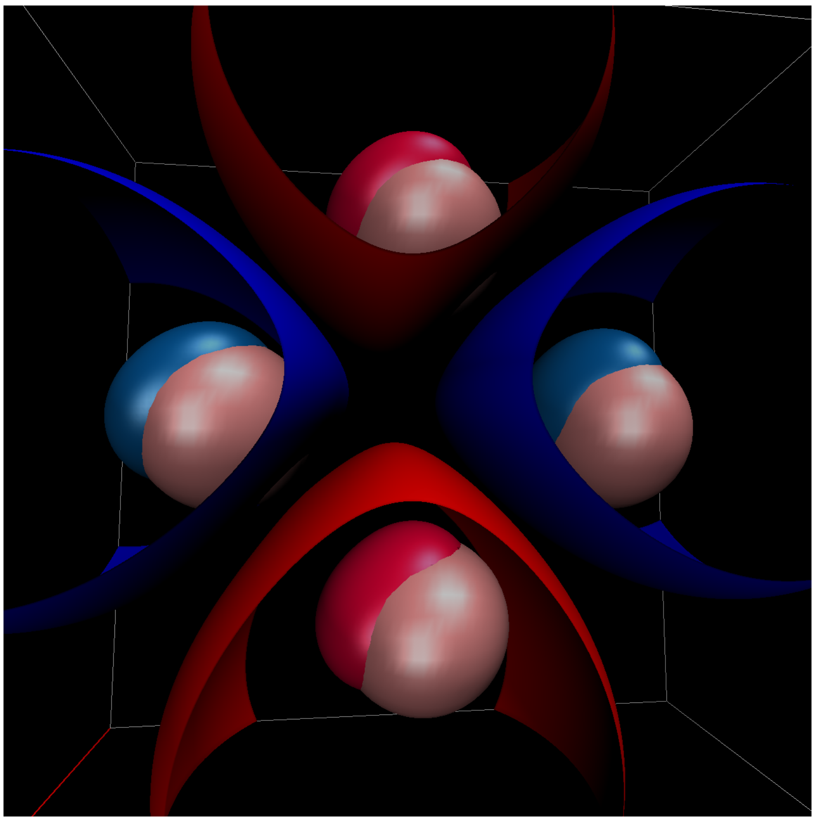


Figure 4.4: DX representation

### 4.3.2 2D ESP plots

From the electrostatic option in PB-AM, a file is created with the following format:

```
# Data from PBAM Electrostat run
# My runname is barnase.x.0.dat
units kT
grid 200 200
axis x 0
origin −51.2204 −51.2204
delta 0.512204 0.512204
maxmin 1.35396 0
   0.2352107      0.2360552      0.2368904      0.2377159
```

In our `tools` directory we have provided a python script for plotting this potential. Change filename within .py file, and the desired output name.

```
>> python potential_plot
```

creates a JPG file of the cross sectioned potential, like the one given below:

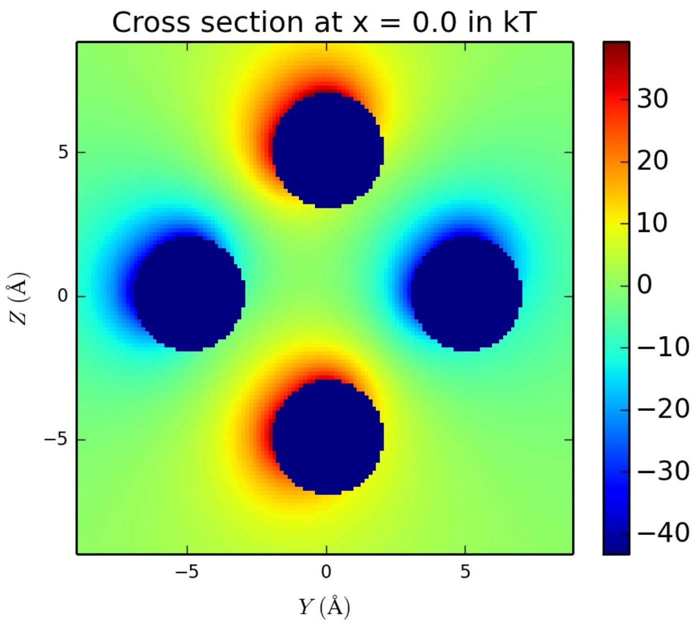


Figure 4.5: Potential plot

### 4.3.3 3D ESP plots

From the electrostatic option in PB-AM, a file is created with the following format:

```
# Data from PBAM Electrostat run
# My runname is electro_map.out and units kT
grid 10 10 10
origin −4 −9 −9
delta 0.8 1.8 1.8
  0.00000    0.00000   −2.90000  −5.899581
```

In our `tools` directory we have provided a python script for plotting this potential. Change filename within .py file, and the desired output name.

```
>> python plot_3d_surf
```

creates many JPG files of the cross sectioned potential, like the one given below:

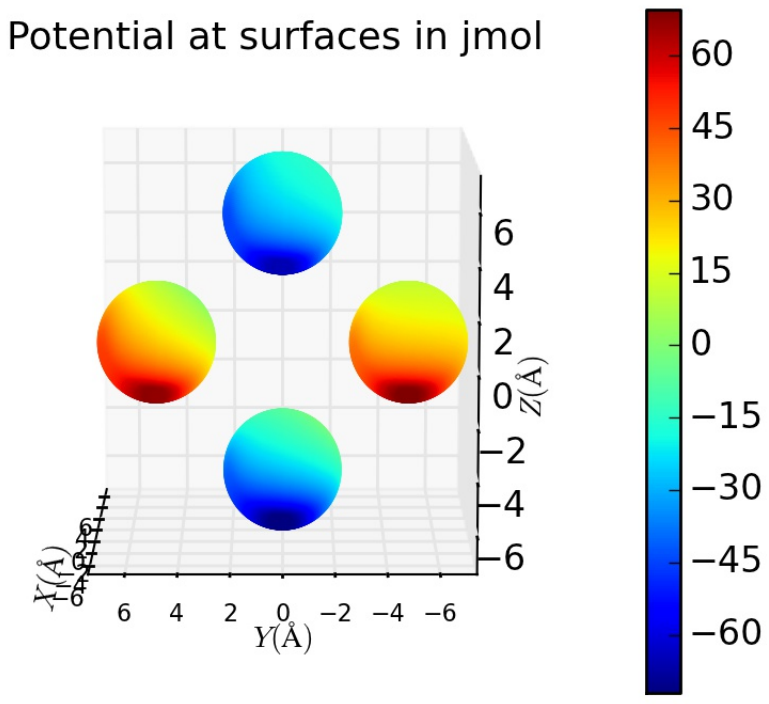


Figure 4.6: Molecule surface potential plot

# Chapter 5

# Common Errors

## 5.1 Errors while reading input file

Our file reader catches some errors, like files not exisiting or being unable to open them. Look at the verbose stream of the program to make sure all your flags are being caught, and check the stream for errors as well.

## 5.2 Segmentation Fault while reading input file

Our file reader is not very robust. Make sure there is only a single space between keywords and options. Make sure that all options are specified for a given keyword.

## 5.3 Initial configuration errors

Many issues may arise if your molecules are overlapping, which is not allowed in the PB solvers' models. The center of the molecule will be placed at the positions given by each XYZ file. Check the printed out PQR file for the initial configuration, which you can load into VMD. Try changing the xyz file(s). This error may also appear if the box length specified with the pbc keyword is too small. Try increasing the box length.