Multigrid Calculations

Common input conditions:

1. **Boundary condition:** Multiple Debye Huckel condition
2. **Type of PBE:** Non linear Poisson Boltzmann Equation
3. **Charge Mapping:**Cubic B-spline discretization (mapped to nearest and next nearest neighbours)
4. **Centre of the Grid: the molecule of interest**
5. **Solvent Dielectric Constant = 78.54**
6. **Solute molecule Dielectric Constant = 2.00**
7. **Radius of Solvent Molecule(in Å) = 1.40**
8. **Srfm:** Smoothed molecular surface definition Model used to construct the dielectric and the ion accessibility coefficients. Link to the documentation: link
9. **Swin: 0.30** Specify the size of the support (i.e., the rate of change) for spline-based surface definitions. (in accordance with srfm)
10. **Temperature = 298.15**
11. **sdens:** Number of quadratures per $Å^2$ to use in calculations for surface terms=10.00

1. **Input conditions:**

Coarse grid lengths 101.6*115.23*121.24
Fine grid lengths 80*88*91

Final Result:

Polar Solvation energy = $-2.733*10^4$ kJ/mol

```
PRINT STATEMENTS

print energy 1 (ion_solv) - 2 (ion_ref) end
  Local net energy (PE 0) = -4.358083172873E+04 kJ/mol
  Global net ELEC energy = -4.358083172873E+04 kJ/mol

print energy 3 (undissc_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.624686874855E+04 kJ/mol
  Global net ELEC energy = -1.624686874855E+04 kJ/mol

print energy 1 (ion_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.244755384292E+04 kJ/mol
  Global net ELEC energy = -1.244755384292E+04 kJ/mol

print energy 1 (ion_solv) - 2 (ion_ref) - 3 (undissc_solv) + 4 (undissc_ref) end
  Local net energy (PE 0) = -2.733396298017E+04 kJ/mol
  Global net ELEC energy = -2.733396298017E+04 kJ/mol
```

2. **Input conditions:**

Coarse grid lengths 100*100*100
Fine grid lengths 75*75*75

Final Result:

Polar Solvation energy = $-3.0100*10^4$ kJ/mol

```
PRINT STATEMENTS

print energy 1 (ion_solv) - 2 (ion_ref) end
  Local net energy (PE 0) = -4.812833501934E+04 kJ/mol
  Global net ELEC energy = -4.812833501934E+04 kJ/mol

print energy 3 (undissc_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.802780340704E+04 kJ/mol
  Global net ELEC energy = -1.802780340704E+04 kJ/mol

print energy 1 (ion_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.342680982858E+04 kJ/mol
  Global net ELEC energy = -1.342680982858E+04 kJ/mol

print energy 1 (ion_solv) - 2 (ion_ref) - 3 (undissc_solv) + 4 (undissc_ref) end
  Local net energy (PE 0) = -3.010053161230E+04 kJ/mol
  Global net ELEC energy = -3.010053161230E+04 kJ/mol
```

3. **Input conditions:**

Coarse grid lengths 150*150*150
Fine grid lengths 75*75*75

Final Result:

Polar Solvation energy = -3.0101*10^4 kJ/mol

```
PRINT STATEMENTS

print energy 1 (ion_solv) - 2 (ion_ref) end
  Local net energy (PE 0) = -4.812838514591E+04 kJ/mol
  Global net ELEC energy = -4.812838514591E+04 kJ/mol

print energy 3 (undissc_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.802780302997E+04 kJ/mol
  Global net ELEC energy = -1.802780302997E+04 kJ/mol

print energy 1 (ion_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.342679187852E+04 kJ/mol
  Global net ELEC energy = -1.342679187852E+04 kJ/mol

print energy 1 (ion_solv) - 2 (ion_ref) - 3 (undissc_solv) + 4 (undissc_ref) end
  Local net energy (PE 0) = -3.010058211594E+04 kJ/mol
  Global net ELEC energy = -3.010058211594E+04 kJ/mol
----------------------------------------
```

4. **Input conditions:**

Solvation with NPBE

Final Result:

Polar Solvation energy = -3.0101*10^4 kJ/mol

```
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PRINT STATEMENTS

print energy 1 (ion_solv) - 2 (ion_ref) end
  Local net energy (PE 0) = -4.812838514591E+04 kJ/mol
  Global net ELEC energy = -4.812838514591E+04 kJ/mol

print energy 3 (undissc_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.802780302997E+04 kJ/mol
  Global net ELEC energy = -1.802780302997E+04 kJ/mol

print energy 1 (ion_solv) - 4 (undissc_ref) end
  Local net energy (PE 0) = -1.342679187852E+04 kJ/mol
  Global net ELEC energy = -1.342679187852E+04 kJ/mol

print energy 1 (ion_solv) - 2 (ion_ref) - 3 (undissc_solv) + 4 (undissc_ref) end
  Local net energy (PE 0) = -3.010058211594E+04 kJ/mol
  Global net ELEC energy = -3.010058211594E+04 kJ/mol
---------------------------------------
```

Geometric flow solvation model

Note: Since this formulation ignores ions, it is not valid for our case. I used it just to experiment.

Input conditions:

1. Grid spacing: 0.25*0.25*0.25
2. Bulk concentration of solvent = 0.003346 Angstrom^-3
3. Error Tolerance = 10^-6
4. Microscopic surface tension = 0.0001 kcal mol^{-1} $Å^{-2}$

```
totalSolv:      -21437  nonpolar: 0.434522      electro: -21437.4

  Global net energy = -2.143697386994E+04
  Global net ELEC energy = -2.143740839161E+04
  Global net APOL energy = 4.345216667319E-01
```

Units = kJ/mol

Boundary Element Method (Tree Code Accelerated Boundary Integral)

Inputs:

1. **Temperature=298.15**

2. **MAC:** Multipole Acceptance Criterion, basically a criterion used to choose one of the direct summation or Taylor expansion methods= 0.8

3. **Mesh:** Ses nanoshaper

4. **Pdie:** Dielectric of solute molecule = 2.0

5. **Sdens:** Number of quadratures per $Å^2$ to use in calculations for surface terms. = 10.00

6. **Sdie:** Solvent dielectric constant=78.54

7. **Srad:** Solvent radius=1.40

8. **Tree_n0:** max number of particles in a treecode leaf=500

9. **Tree_order:** taylor expansion order=300

Solvation and free energy of dissociated PAA

```
Solvation energy = -40687.501371 kJ/mol
Free energy = -64761.241961 kJ/mol

The max and min potential and normal derivatives on elements area:
potential 83.595779 -51.684367
norm derv 7682.608618 -12914.852928

The max and min potential and normal derivatives on vertices area:
potential 80.997097 -49.864882
norm derv 7326.229457 -12482.210512



Returning to APBS caller...

Solvation energy and Coulombic energy in kJ/mol...

  Global net ELEC energy = -4.068750137145E+04
  Global net COULOMBIC energy = -2.407374058906E+04
```

Solvation energy and free energy of undissociated PAA using SES Nanoshaper

```
Solvation energy = -6863.645516 kJ/mol
Free energy = -12177.666597 kJ/mol

The max and min potential and normal derivatives on elements area:
potential 108.788696 -32.333650
norm derv 21049.275816 -9977.109517

The max and min potential and normal derivatives on vertices area:
potential 75.885324 -31.774559
norm derv 14221.388409 -4443.465186



Returning to APBS caller...

Solvation energy and Coulombic energy in kJ/mol...

  Global net ELEC energy = -6.863645516173E+03
  Global net COULOMBIC energy = -5.314021080352E+03
```

Therefore, Polar solvation energy = -4*10^4+6.86*10^3

= -3.382*10^4 kJ/mol