Tools for DDSCAT calculation of charged particles

Author: Frantisek Kundracik

The scattering properties of surface charged particles seems to be very interesting. The surplus surface charge influences the electric conductivity near the particle surface, and finally the complex refraction index of the surface layer.

This set of tools enables:

1. To read the DDSCAT shape-file (shape.dat) and to reconstruct the 3D model of the particle.

2. To calculate the electric field and the surplus electric charge at the particle surface, if the particle potential is given.

3. To smooth the calculated surface charge (suppression of the effects caused by the discretisation of the particle model).

4. To make the charged surface layer thicker – the goal is the lowering the refraction index of the surface layer.

5. To calculate the electric conductivity and refractive index of the surface layer, the calculation is based on Drude model.

6. To prepare all files needed by DDSCAT-program (configuration, shape and material files). As a result, DDSCAT can be used for calculations of scattering properties of charged particles.

7. To visualize the charge distribution on the particle surface.

9. To create a plane cut of the particle and too see the charge distribution inside the surface layer.

10. To modify automatically the wavelength and/or the effective radius in the ’ddscat.par’ file. This allows to automatize the computation using batch-scripts.

The tools expects, that the user has prepared all the files needed for the DDSCAT calculation of an uncharged particle (ddscat.par, shape.dat and material description files). The tools imports these files and prepares new set of them that corresponds to the charged particle.

Content

Instalation

Windows:

The installation procedure is quite simple. In Windows you can use compiled executables:

1. Unpack charged_ddscat_window.zip into any folder.
2. Copy ddscat.exe (from http://ddscat.wikidot.com/windows) tool to the same folder.

Linux:

In Linux you need compile the tools:

1. Unpack charged_ddscat_source.zip into any folder.
2. Compile all C++ files. All tools are single C++ files, no makefile is needed. Use any C++ compiler, like GCC or CodeBlocks.
3. Download and compile DDSCAT software (from http://ddscat.wikidot.com/downloads) and copy the compiled 'ddscat' executable to the same folder where the charged_ddscat tools are located.

Step-by-step instructions

To test your freshly installed tools and to make you more familiar with the tools, we provide a demo-particle model. It is already installed in the same folder, where the tools are (see "Installation" chapter)

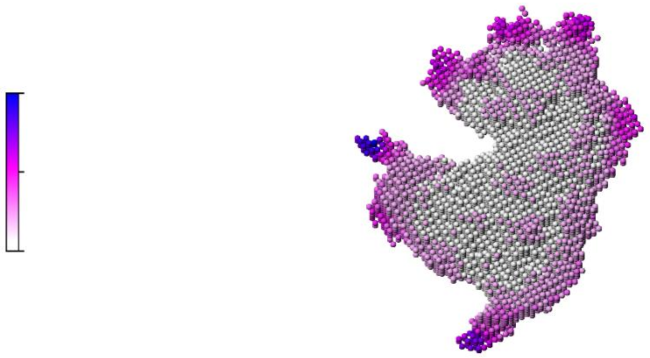
1. At first we will test your DDSCAT program. Look into the folder containing the tools. You will see the "shape.dat" file (description of an irregular particle), "ddscat.par" file (parameters for the ddscat program) and "sio2.dat" file (material file of the particle). These three files are needed to run the DDSCAT program. Go to the folder containing the tools and run the DDSCAT program. If everything is OK, no error-messages will be displayed and new files (target.out, w000r000.avg, w000r000k000.fml, w000r000k000.sca, mtable, qtable and qtable2) will be created. Look into "w000r000.avg" file and you should find following rows:

```
Results averaged over    1 target orientations
                  and    2 incident polarizations
         Qext         Qabs         Qsca      g(1)=<cos>  <cos^2>      Qbk        Qpha
JO=1:  5.1278E-04  5.1279E-04  1.4022E-09  2.0205E-04 4.0243E-01 1.6704E-10  7.2820E-03
JO=2:  3.2825E-04  3.2825E-04  9.0573E-10  1.9692E-04 3.9746E-01 1.0114E-10  5.6647E-03
mean:  4.2051E-04  4.2052E-04  1.1540E-09  2.0004E-04 3.9746E-01 1.3409E-10  6.4733E-03
```

2. The second step is the calculation of the normalised surface charge density at the particle surface. Look into "laplace.par" file for the parameters of the LAPLACE-tool. Run the "laplace" program. It takes some time, but finally three data files are generated: "shape.3d" (compressed shape file), "shape.3c" (compressed charge file) and "materials.dat" (number of materials found). For more information consult the chapter "1 Surface charge calculation".
The calculation of the surface charge can be time consuming, but has to be done only once for each particle. The calculated charge density can be later automatically scaled to any surface potential and any particle size.

3. Next step is the smoothing of the charge distribution at the particle surface. Look into the “chargeavg.par” file for the parameters of the smoothing. Run the “chargeavg” program. New files are generated: “shape.3m” (compressed charge distribution) and “charge.dat” (calibration data). Consult the chapter “2 Averaging the surface charge” for more information.

4. Now we can eventually investigate the surface charge distribution at the particle surface. The CHARGE2BMP tool creates a BMP-image of the particle. Look into the “charge2bmp.par” file for the parameters of the visualisation. Run the “charge2bmp” program. As a result, a “shape.bmp” file is produced:



   The colour scale of the picture represents the charge density. See chapter “4 Charge density viewer” for more information.

5. Now we are ready to prepare new configuration files (containing information about the charged particle) for the DDSCAT program. Look into the “charge2ddscat.par” file to see the parameters of the conductivity model (Drude). Then run the “charge2ddscat” program. As a result, new folder “charged” was created. In this folder you can find: “shape.dat” file (particle shape and composition description), “ddscat.par” file (parameters for the DDSCAT program) and finally eight material files “mat001.dat” – “mat008.dat” (material parameters corresponding to various levels of the charge density). Consult the chapter “3 Creation of new files for DDSCAT” for more information.

6. The final step is the run of the DDSCAT program for charged particle. Simple (and not very clever) method is as follows: copy the “ddscat” executable into the freshly created “charged” folder and run the “ddstat” program. Look into the resulting “w000r000.avg” file and you should find following lines:

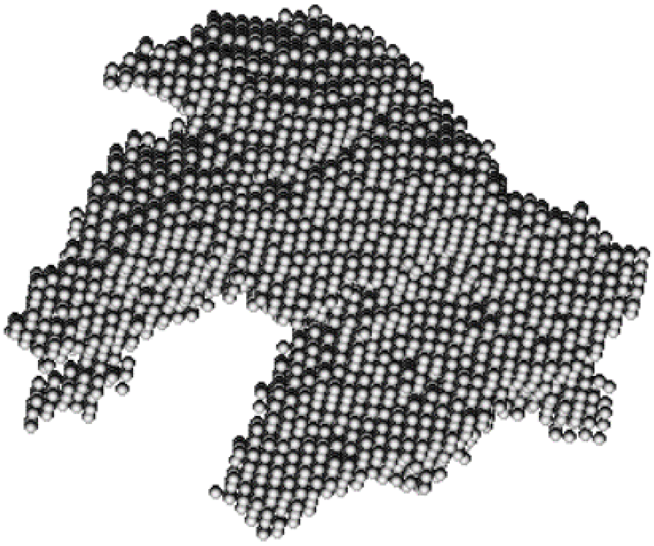
```
Results averaged over    1 target orientations
                  and    2 incident polarizations
         Qext        Qabs        Qsca      g(1)=<cos>  <cos^2>      Qbk        Qpha
JO=1:  2.3408E-03  2.3408E-03  1.4223E-09  2.9986E-04 4.0243E-01 1.6938E-10  7.2456E-03
JO=2:  1.4350E-03  1.4350E-03  9.1917E-10  2.2775E-04 3.9752E-01 1.0273E-10  5.6667E-03
mean:  1.8879E-03  1.8879E-03  1.1707E-09  2.7155E-04 3.9752E-01 1.3606E-10  6.4562E-03
```

   Compare these results (charged particle) with results obtained in step 1 (non-charged particle): you can see that the absorption cross-section (Qabs) is significantly higher for the charged particle.

   Consult the chapter “6 The ‘ddscat.par’ file modifier” for more efficient batch-methods of the calculations.

Particle model

The tools were tested on an irregular shape morphologically identical with the particle captured by NASA spacecraft:



The numerical model of the particle has the linear size of 45 voxels and the volume of the particle is 9649 voxels (elementary dipoles). The computations were made on a standard PC equipped with Intel I5 processor.

1. Surface charge calculation (laplace.exe)

This tool imports the 'shape.dat' file (input file for DDSCAT) first. Than it calculates (using the Laplace equation) the surface charge density of the particle assuming standard surface potential of 1V and standard particle size (distance between dipoles) of 1 nm. Such way calculated charge density can be easily scaled to other surface potentials and particle sizes.

Numerical method

The Laplace equation

$$\Delta V(x, y, z) = 0 \tag{1}$$

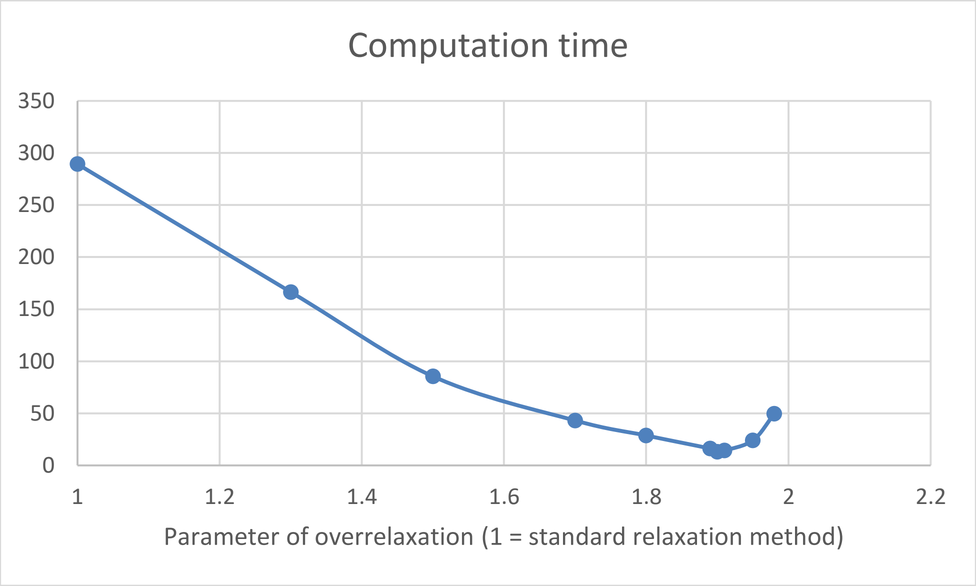
has to be solved in outer space of the particle for boundary conditions $V = V_0$ at particle surface and $V = 0$ at large distances from the particle.

We used a well-known Gauss-Seidel over-relaxation numerical method in simple equidistant mesh in the 3D-space with discretization step h. The indices of the mesh points are $i, j, k = 1, 2, \ldots, N$.

The Gauss-Seidel over-relaxation method leads to the iteration scheme

$$V_{i,j,k}^{new} = (1-\lambda)V_{i,j,k}^{old} + \frac{\lambda}{6}\left(V_{i+1,j,k}^{old} + V_{i-1,j,k}^{old} + V_{i,j+1,k}^{old} + V_{i,j-1,k}^{old} + V_{i,j,k+1}^{old} + V_{i,j,k-1}^{old}\right) \tag{2}$$

The optimal value of over-relaxation parameter λ has to be found for each problem type and can be chosen freely in 'laplace.par' file. For our irregular particle we have found following dependence of the computation time on the over-relaxation parameter value:



We have found that for our problem a value of 1.9 is optimal and ca 20-times shorter computation time in comparison to the classic relaxation method can be achieved.

The numerical methods, in generally, calculate the electric field in a limited space. Classical zero-value Dirichlet boundary condition leads to escalated electric field at the surface of the particle in comparison to that field of a particle placed in free space. To avoid this problem, we model the field at the outer boundary by a field of a sphere charged to the same charge as the particle:

$$V(x,y,z) = \frac{1}{4\pi\varepsilon_0} \frac{Q}{\sqrt{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}} \tag{3}$$

where x_0, y_0 and z_0 is the position of the center of the particle. Of course, the value Q remains unknown until the Laplace equation is not solved. So the process is iterative:

1. The potential of the particle voxels is set to V_0. The value of Q is estimated using the capacity of the volume equivalent sphere $Q = 4\pi\varepsilon_0 R_{ekv} V_0$

2. The potential at the outer boundary is set using relation (3)

3. The potential field is solved using scheme (2)

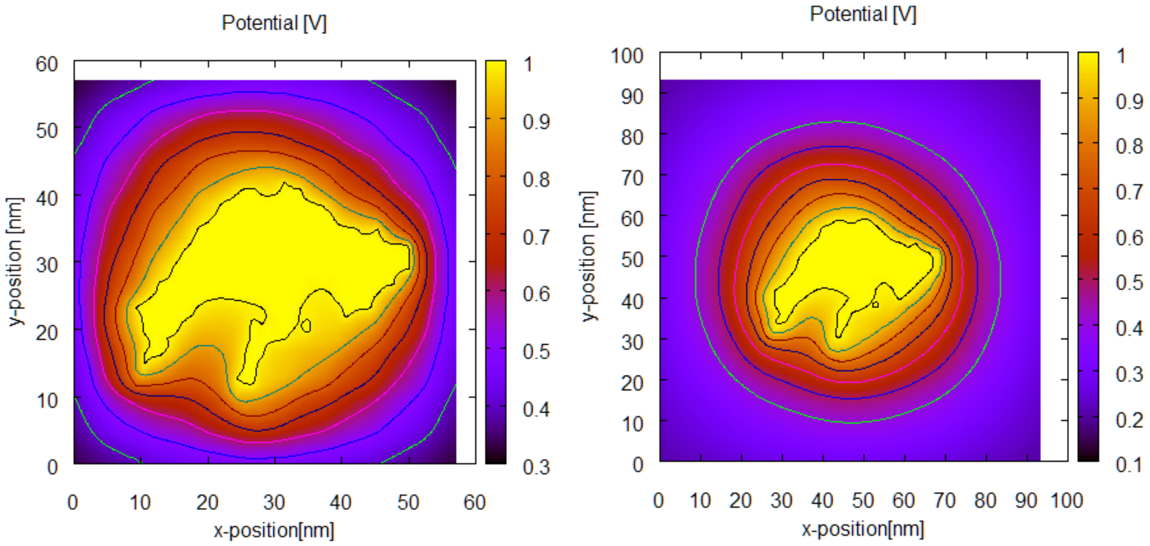
4. The volume charge density of the voxels at the particle surface is calculated:

$$\rho(x,y,z) = \varepsilon_0 \operatorname{div} \vec{E} == \frac{\varepsilon_0}{h^2}\left(V_{i+1,j,k} - V_{i-1,j,k} + V_{i,j+1,k} - V_{i,j-1,k} + V_{i,j,k+1} - V_{i,j,k-1}\right) \tag{4}$$

5. New value of the total surface charge Q is found.

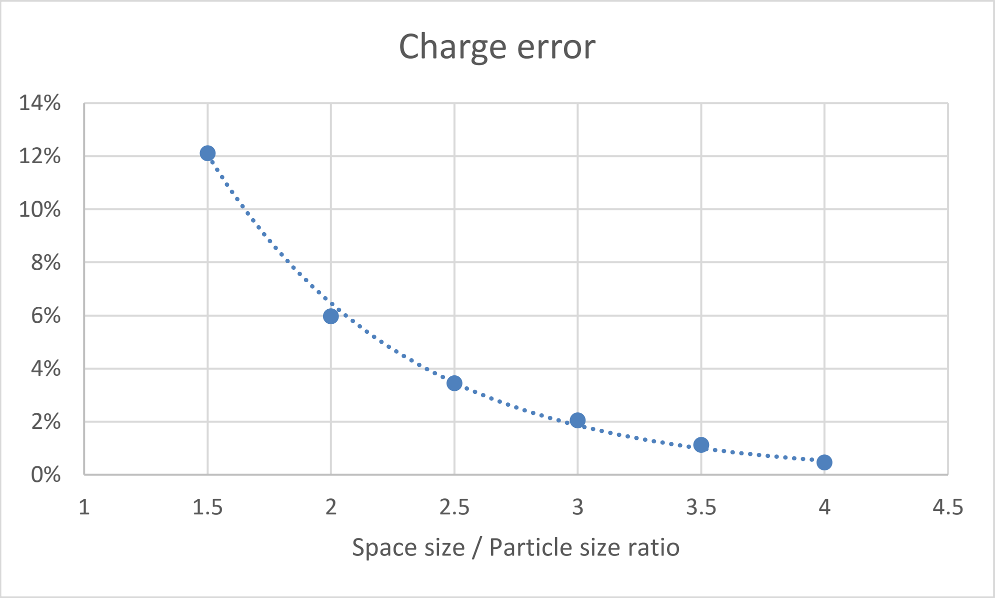
6. Steps 2 – 5 have to be repeated until the value of Q relaxes to the terminal value.

This trick enables to choose much smaller computation space and to achieve dramatically faster computations. The obtained potential field (z=0 cut) of a realistic irregular particle is shown in next figure:



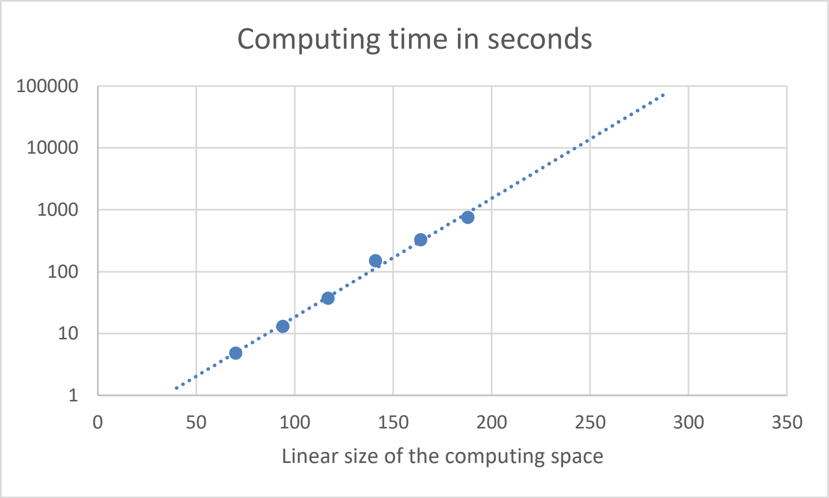
Left: Computational space size is 1.25-times larger than the particle size.
Right: Computational space size is 2.0-times larger than the particle size.

The dependence of the error in calculated total surface charge on the ratio of the computation space to the particle size is in the figure:



Of course, the error strongly depends on the particle shape. For nearly spherical particles it is significantly lower than one shown in the figure. So, the value of about 2 is optimal for most particles, for strongly non-spherical particles the value of about 2.5 - 3 seems to be optimal and can be set in 'laplace.par' file. One has to realize that the distribution of the surface charge is modelled in DDSCAT by a set of discrete materials (e.g. 32 materials representing 32 levels of the charge density), so the precision of the calculated charge density of few % is acceptable.

Larger values of the above mentioned ratio can lead to dramatically higher number of the mesh points and to an enormous computing time:



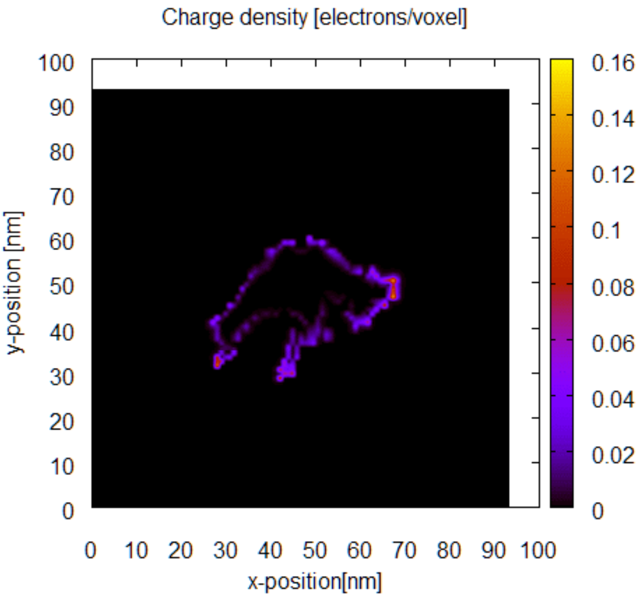
It is clear, that relatively short computing time up to 200 s can be achieved for the computing space up to 150 x 150 x 150 voxels = 3.3 millions of voxels. For “space size / particle size” ratio of 2 it means, that nearly spherical particle can be built from up to 0.22 million of voxels and its diameter can be up to 75 voxels.

We also have tested the computation time for a spherical particle with radius of 36 nm (diameter of 73 voxels) for “space size / particle size” ratio of 2. The computation time was 119 s, calculated surface charge was found to be 25.3 electrons/V. The analytically calculated value is 25.0 electrons/V, so the error of the calculation was ca 1%.

Larger (with higher amount of voxels) particles can be processed, but one has to be aware, that doubling of the linear size results in 2 orders of magnitude longer computation time (ca 5 hours for 300 x 300 x 300 = 26 millions of voxels). Such situation corresponds to the surface charge calculation on a sphere with the radius of 60 voxels at “space size / particle size” ratio of 2.5. The total number of voxels (dipoles) of such sphere reaches ca 1 million, what is currently also the limit of the DDSCAT software.

The computing time for our model particle and “space size / particle size” ratio of 2 was 13 s.

The approximate surface charge distribution (z=0 cut) for 10 V particle potential is:



It is visible that the charge is concentrated near sharp edges. The total surface charge of the 45 nm sized particle charged to 10 V was found to be 108 electrons.

2. Averaging of the surface charge (chargeavg.exe)

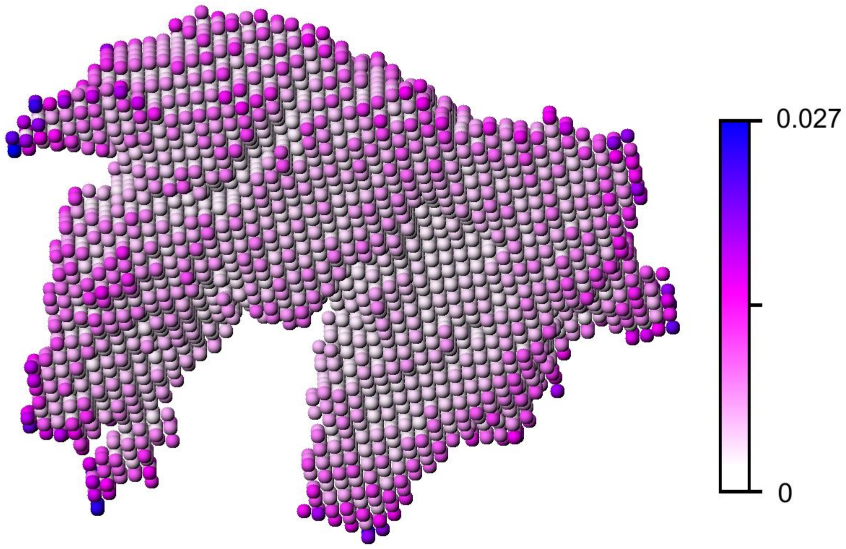
There are two good reasons why to smooth the calculated charge density. Firstly, the discretisation model of the particle leads to the presence of layers of voxels (dipoles). The charge density on the edges of such layers is higher than in the rest of the layers. Secondly, high charge density can lead to high refractive index of the surface layer and to problems in DDSCAT precision. That's why we have implemented an averaging routine. Its principle is simple. The charge from each voxel is distributed into that neighbouring voxels, which are closer than certain value (averaging parameter).

The averaging has two steps.

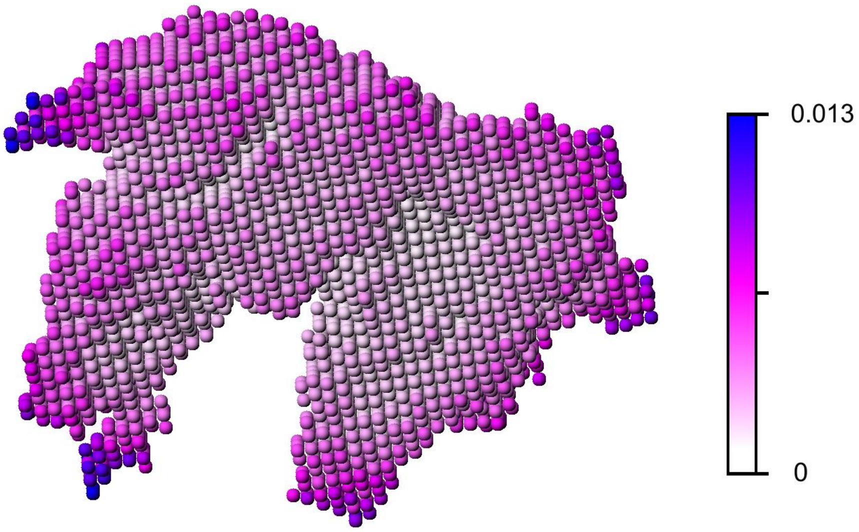
1. The averaging of the charge on the surface of the particle. The charge is averaged between surface voxels only. The parameter (radius of the smoothing r_s>0measured in voxel size) can be set freely in 'chargeavg.par' file.
2. The spreading the charge from the surface voxel into the interior of the particle. The result is, that the surface layer gets thicker and the charge density gets lower (more suitable for DDSCAT). The parameter (radius of the smoothing r_s>0 measured in voxel size) can be set freely in 'chargeavg.par' file.

We have implemented two averaging modes. The first one distributes whole charge from the central surface voxel evenly into all neighbouring voxels (including the central voxel). This mode works well on smoother particles. The second mode distributes only a (1–1/r_s)-part of the charge from the central surface voxel into neighbouring voxels. This mode gives better results on particles having sharp edges and/or spikes and leads also to the gradually decreasing charge density from the surface to the centre of the particle.

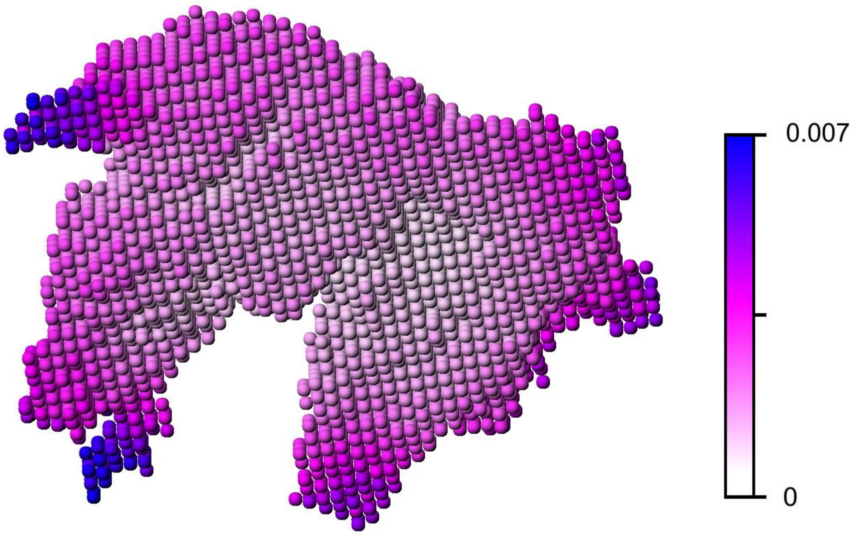
The result of the averaging can be seen on next figures.



Charge density (in electrons per voxel) on the surface of a particle charged to 1V.
Surface averaging parameter: 0 (no averaging), volume averaging parameter: 0 (no averaging)



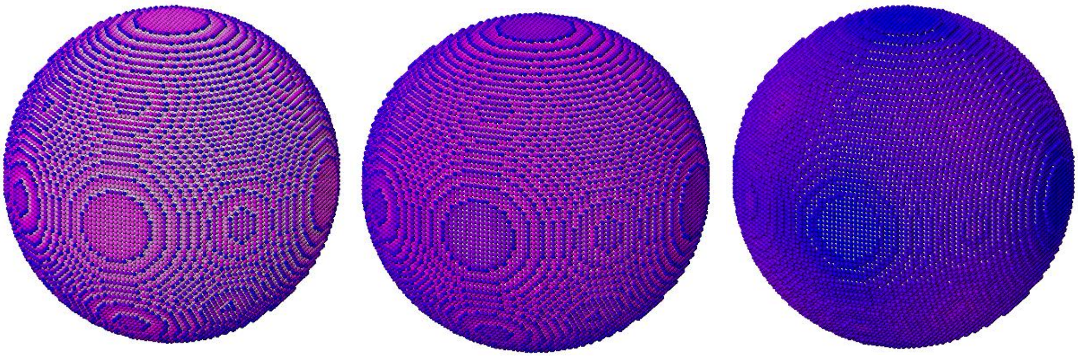
Charge density (in electrons per voxel) on the surface of a particle charged to 1V. Surface averaging parameter: 3, volume averaging parameter: 0 (no averaging), averaging mode: 2 (highly irregular particle)



Charge density (in electrons per voxel) on the surface of a particle charged to 1V. Surface averaging parameter: 3, volume averaging parameter: 3, averaging mode: 2 (highly irregular particle)

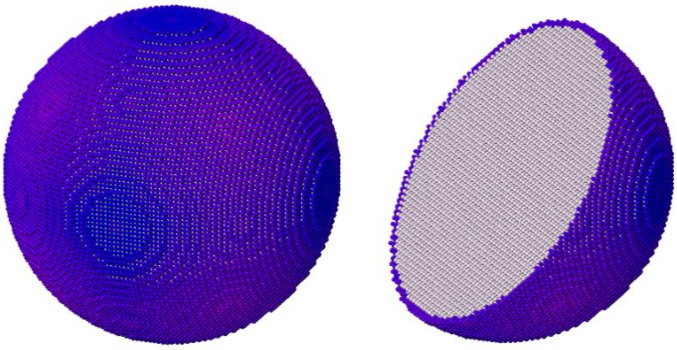
It is clearly visible, that averaging leads to lowering of the extremal values of the charge density. Of course, some degradation of the spatial resolution must be accepted, after the averaging was applied.

The whole smoothing process can be nicely shown on a charged sphere. In the next figure it is visible, that the discretisation of a sphere leads to the charge accumulated on edges of the layers. This irregular charge distribution on smooth surfaces is only an artefact caused by the discretisation of the particle. Surface charge averaging (mode 1 – smooth particle) leads to smoother surface charge distribution.

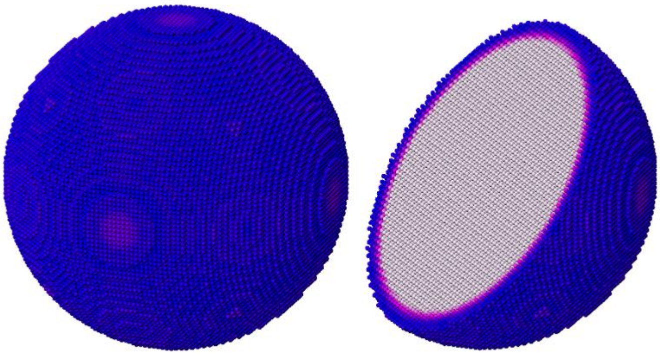


Charge on the surface of a sphere for surface smoothing parameter value of 0 (left), 3 (middle) and 5 (right), averaging mode: 1 (smooth particle)

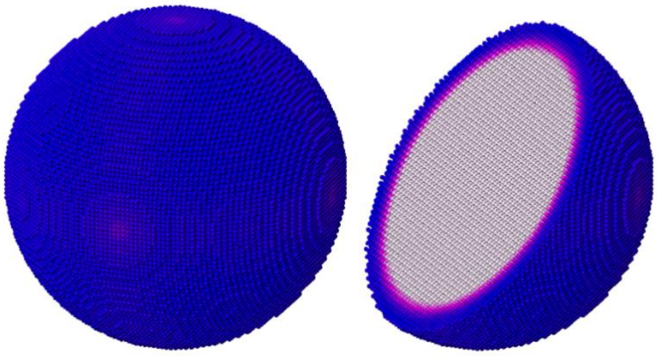
Applying the volume smoothing, the charge spreads also into interior layers of the particle model. The result is, that the charged layer gets thicker and the charge density gets lower. In the next figures it is shown the interior of a sphere with various values of the volume smoothing parameter applied.



Charge on the surface and inside of a sphere. Surface smoothing parameter = 5, volume smoothing parameter = 0 (no smoothing), averaging mode: 1 (smooth particle)

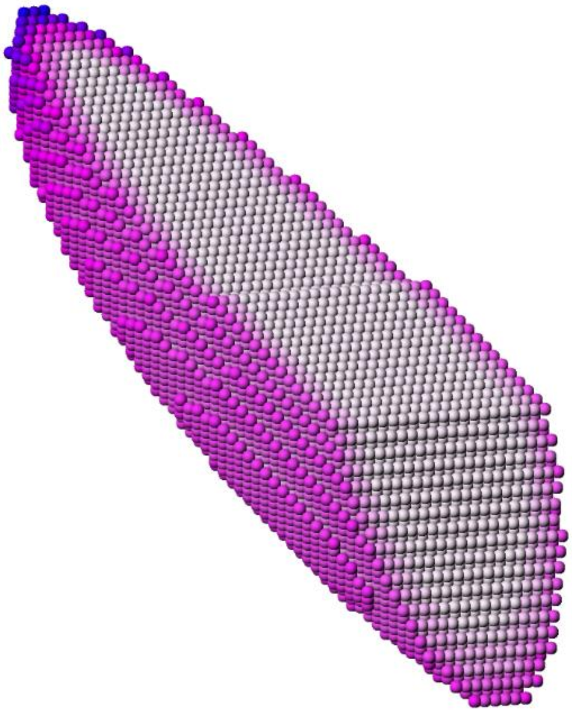


Charge on the surface and inside of a sphere. Surface smoothing parameter = 5, volume smoothing parameter = 3, averaging mode: 1 (smooth particle)



Charge on the surface and inside of a sphere. Surface smoothing parameter = 5, volume smoothing parameter = 5, averaging mode: 1 (smooth particle)

Use of the smoothing mode 2 leads to gradually decreased charge density in the inner layers. This can be useful in some cases, as the DDSCAT is sensitive to fast changes in refractive index, too. Next figure shows the charge distribution in an elongated ellipsoid after charge smoothing (mode 2).



Charge on the surface and inside of an ellipsoid (double cut). Surface smoothing parameter = 3, volume smoothing parameter = 3, averaging mode: 2

Besides the smoothing parameters, in “chargeavg.par” file we can choose also the output number of levels of the charge density. The higher is the number of levels, the smoother is the charge distribution, but the higher is the number of materials that DDSCAL will process. Be aware, that the standard DDSCAT compilation accepts 9 materials only.

3. Creation of new files for DDSCAT (charge2ddscat.exe)

Modifying the 'shape.dat' and 'ddscat.par' files

The last step is the creation of new files for DDSCAT software. The particle potential and the parameters of the conductivity model are specified in 'charge2ddscat.par' file.

The creation of new "shape.dat" and "ddscat.par" files is simple – all data (discretised charge density in the voxels) were already collected in previous steps. The "ddscat.par" undergoes following changes:

1. Number of materials is changed. New (much numerous) set of materials describes all original (uncharged) materials used in "shape.dat", but charged to all discrete levels (including no charge).

2. Wavelengths and effective radii settings are modified in that way, that only the first value is used. The reason is, that any change in wavelength and/or effective radius results in the change of material properties of the surface layer. So, we can't use the sweep-ability of DDSCAT. Instead of that, for each wavelength/radius combination we have to run 'charge2ddscat' tool and to create new set of files for DDSCAT.

The main job of the 'charge2ddscat' tool is to create a new set of material files. If the number of (uncharged) materials in "shape.dat" is N_1 and the number of charge levels (see 'chargeavg' description above) is N_2, then the total number of new materials is N_1N_2. Be aware, that the standard DDSCAT compilation allows 9 materials only. So you have to use a specially compiled version allowing up to 256 materials. If you use the standard version of DDSCAT, you can use for example 8 charge levels (see 'chargeavg') if only 1 material is present in "shape.dat" or 4 charge levels if 2 materials are present in "shape.dat".

The physical concept of the refractive index of charged material is described as follows.

Physical concept of refractive index of the charged surface layer

The surplus charge can move on the particle surface. To incorporate the surface charge into DDSCAT, we assume, that the surface charge is physically located in the surface layers of the particle model and that it can move independently on the particle material. Such approach is fully equivalent to the situation, when the added charge is moving on the surface, the only approximation is the geometrical location of the added charge – it is located slightly deeper in the particle. So, the precision of this approximation is given by the precision of the original particle model (number of discrete dipoles) only.

The average movement of the surface charge carriers (electrons) in an external electric field is given by the equation

$$\dot{v} = \frac{q}{m} E - \gamma v$$

Where *m* and *q* are mass and charge of an electron, Υ is the dumping coefficient inversely proportional to the relaxation time, *v* is the velocity and *E* is the external electric field.

Assuming the harmonic excitation

$$Ee^{-i\omega t}$$

we can obtain

$$v = \frac{q/m}{\gamma - i\omega} E$$

If ρ is the volume charge density (in C/m^3) of the surplus charge, the electric current density (in A/m^2) is

$$j = \rho v = \frac{\rho q}{m} \frac{1}{\gamma - i\omega} E$$

And the electric conductivity (in S/m) of added charge carriers is

$$\sigma = \frac{\rho q}{m} \frac{1}{\gamma - i\omega}$$

If $n = n' - i\, n''$ is the complex refractive index and $\varepsilon = n^2$ is the complex dielectric constant of the particle, the additional conductivity σ influences the complex permittivity (ε_0 is the permittivity of free space) by:

$$\varepsilon_{new} = \varepsilon - i \frac{\sigma}{\omega \varepsilon_0}$$

as can be directly seen from well-known wave equation

$$0 = \Delta E + i\omega\mu_0\sigma\, E - \omega^2 \varepsilon\varepsilon_0\mu_0 E = \Delta E - \omega^2 \mu_0 \varepsilon_0 \left(\varepsilon - i \frac{\sigma}{\omega\varepsilon_0} \right) E$$

So, the new complex effective refractive index of the particle is

$$n_{new} = \sqrt{\varepsilon_{new}} = \sqrt{\varepsilon - \frac{i}{\omega\varepsilon_0} \frac{\rho q}{m} \frac{1}{\gamma - i\omega}}$$

The dumping coefficient Υ we estimate by the relation

$$\gamma = \alpha \frac{k_B T}{\hbar}$$

as this formula was found to be valid in wide range of materials. The empirical dissipation coefficient α is usually close to 1.

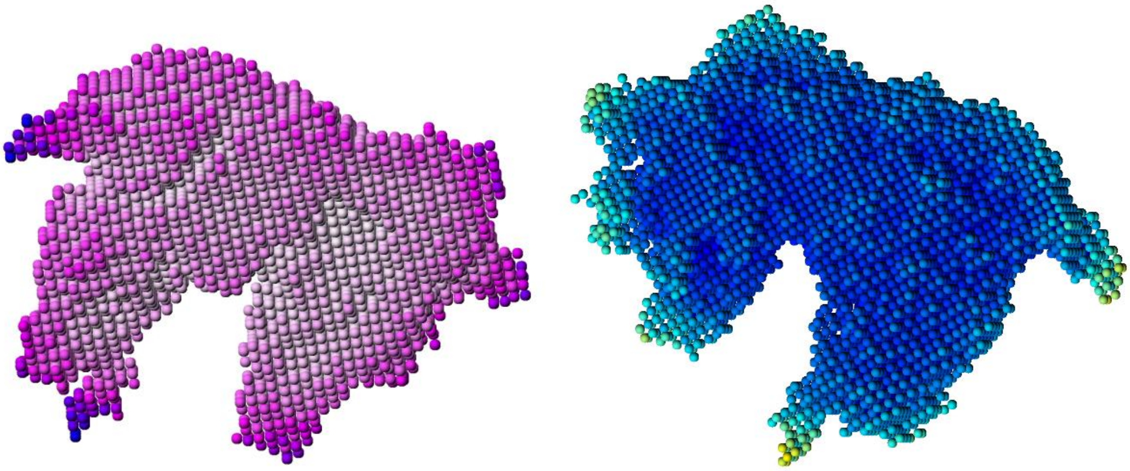
Creating new material files

In each (uncharged) material file there is a table of complex refractive indices (or dielectric constants) for various wavelengths. Each row is read and for given wavelength and given charge density new complex refractive index is calculated by the method described above. Then corresponding number of new material files is written.

4. Charge density viewer (charge2bmp)

This tool serves for the visualization of the charge density in Windows Bitmap (BMP) format. The picture is written to the 'shape.bmp' file. Both the spatial orientation of the particle (Euler's angles) and the colour palette can be set in 'charge2bmp' file.

In ‘charge2bmp.par’ file we can set three RGB-colours that correspond to the zero-level, half- level and maximum values of the charge density. As an example, (255, 255, 255)-(255, 0, 255)-(0, 0, 255) means that uncharged area is white, partly charged area is violet (magenta) and fully charged area is shown in blue colour (see the next figure). Another example is (0, 0, 255)-(0, 255, 255)-(255, 255, 0), the blue – cyan – yellow palette. The optional gamma colour correction can be set in ‘charge2bmp.par’ file.



Charge on the surface of a particle. Left: front side of the particle in white-magenta-blue palette. Right: back side of the particle in blue-cyan-yellow palette (gamma correction = 0.75).

5. Particle cutter (cut3d)

This program enables to create an undercut of the particle and to see its interior using charge2bmp tool. The orientation (x-axis cut, y-axis cut and z-axis cut) of the cutting plane has to be set as command-line parameters. A script cut.cmd (Windows) can be used for easy creation of the cut. The ‘shape.bmp’ contains the picture of the undercut of the particle.

cut.cmd:

```
echo y|copy shape.3d shape_full.3d
cut3d shape_full.3d shape.3d 1 1 1
charge2bmp
echo y|copy shape_full.3d shape.3d
start shape.bmp
```

6. The ‘ddscat.par’ file modifier (setddscatpar)

This program substitutes the sweep-ability of the DDSCAT program. As for each wavelength and/or effective radius a new set of materials has to be created, an automatic change of the wavelength and the effective radius in the ‘ddscat.par’ file is needed. This tool changes both these parameters in ‘ddscat.par’ file without touching other parameters/settings. New values of both parameters are to be set as command-line parameters.

As an example, following Windows PowerShell script ‘sweep.ps1’ makes a wavelength-sweep and stores results in separate folders.

sweep.ps1:

```
$wavelength = 50.0
$radii = @(0.01, 0.02, 0.05, 0.07, 0.1, 0.2, 0.5, 0.7, 1)
foreach ($radius in $radii)
{
    .\setddscatpar $radius $wavelength
    .\charge2ddscat
    cd charged
    ..\ddscat
    cd ..
    $name = "charged_"+ $radius
    mkdir $name;
    copy charged\*.* $name
}
```

The script can be run using the command:

```
powershell.exe .\sweep.ps1
```

If the execution of local unsigned scripts is restricted, run the PowerShell as an administrator first and run the command:

```
Set-ExecutionPolicy RemoteSigned
```

After the computations you can eventually prohibit the execution of the local unsigned scripts using the command:

```
Set-ExecutionPolicy Restricted
```

Data files overview

The communication between the user and the tools and between tools mutually is done using the following data files.

Configuration files:

`laplace.par` – settings of the charge computation method (relative size of the computational space, over-relaxation parameter, precision)

`chargeavg.par` – settings of the charge smoothing and discretisation (surface smoothing radius, volume smoothing radius, smoothing mode, number of output charge levels)

`charge2ddscat.par` – settings of the conductivity model (particle potential, temperature, empirical dissipation coefficient)

`charge2bmp.par` – setting of the charge visualisation (relative picture resolution, Euler’s angles of the particle rotation, RGB palette, colour gamma correction)

Data files:

`shape.dat` – DDSCAT shape description file (used as an input of the ‘laplace’ tool and as an output of the ‘charge2ddscat’ tool)

`shape.3d` – compressed shape form file (output of the ‘laplace’ and ‘cut3d’ tools, input of the ‘chargeavg’, ‘cut3d’, ‘charge2bmp’ and ‘charge2ddscat’ tools)

`shape.3c` – compressed shape charge file (output of the ‘laplace’ tool, input of the ‘chargeavg’ tool)

`shape.3m` – compressed shape material file (output of the ‘chargeavg’ tool, input of the ‘charge2bmp’ and ‘charge2ddscat’ tools)

`charge.dat` – maximum charge density found (output of the ‘chargeavg’ tool, input of the ‘charge2ddscat’ tool)

`materials.dat` – number of materials present in ‘shape.dat’ (output of the ‘laplace’ tool, input of the ‘charge2ddscat’ tool)

`field_cut.dat` – potential in z=0 cut in format suitable for GNUplot (output of ‘laplace’ tool)

`charge_cut.dat` – charge density in z=0 cut in format suitable for GNUplot (output of ‘laplace’ tool)

`mat???.dat` – a set of the DDSCAT material description files - refraction indices tables (output of the ‘charge2ddscat’ tool)

`ddscat.par` – DDSCAT settings file (input and output of the ‘charge2ddscat’ and ‘setddscatpar’ tools)

Block diagram of the tools system skeleton