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# GSvit input files

As an input for GSvit, plain text files are used. The most important one is the parameter file (\*.par) which controls all the calculation (number of steps, computational domain sources, etc.). Some additional files can be used e.g. for specifying the geometry of material inside computational domain.

Here follows the documentation for last stable release:

## Parameter file description

### Main computation settings

Keywords are case sensitive. The following keywords can be used in the current version of GSvit (before issuing version 1.0 this means actual version as obtained from SVN, but nearly all the parameters remain same for last issued binaries):

#### **POOL**

*xres yres zres dx dy dz*

Set computation volume dimensions in pixels (xres, yres, zres) and real pixel size - pixel spacing (dx, dy, dz) in meters. To create a 200x200x200 pixel computational volume with pixel spacing of 1 micrometer, set:

POOL

200 200 200 1e-6 1e-6 1e-6

#### **COMP**

*nsteps*

Set total number of computation steps, e.g. to set the number of steps to 100, write:

COMP

100

#### **THREADS**

*nthreads*

Set total number of threads to be used if we are calculating on CPU (not on GPU). Can be -1 for automated detection of number of cores and use of all of them which is also default behavior (since GSvit 1.3). Note that on systems using hyperthreading the virtual cores do not help (use half of available cores at maximum). Generally, FDTD is memory demanding and scaling with number of cores is therefore not linear (memory is the bottleneck), however up to some 8 threads there is significant speedup. You can test this scaling using ./gsvit test 3N, where N is problem size (e.g. 32 means thread test on 200x200x200 voxels). As an example, to set the number of threads to 4, write:

THREADS

4

#### **MATMODE\_CHECK**

*0/1*

Check material settings and if possible, run computation with smaller memory allocation - not

allocating some of the components and using simplified equations (e.g. for nonmagnetic materials or vacuum). This can save up to half computation time or memory requirements. A safe variant if something fails is 0 which is default value (full calculation). This might be necessary for some novel algorithms before they are tested properly, typically algorithms on GPU where this parameter is not recommended for now. An example of use is:

MATMODE\_CHECK

1

## MEDIUM\_LINEAR

*filename*

Use file that consists of binary data representing material, pixel by pixel. File structure is: xres, yres, zres (binary 32-bit integers) of same size of computation volume, followed by four 3D fields of 32-bit floats representing epsilon, sigma, mu and magnetic conductivity. This approach is ideal for including complex or continuously varying geometries. For simple objects, use vector data input (MEDIUM\_VECTOR), which is much simpler to construct.

## MEDIUM\_VECTOR

*filename*

Use file that consists vector material representation, composed from different basic entities (written in an ASCII file). Each entity entry is composed by the following information:

- type of entity (integer): 4 - sphere, 7 - cylinder, 8 - parallelepiped, 12 - tetrahedron, 21 - tetrahedral mesh in Tetgen output format, 22 - Gwyddion height field, 107 - cone
- point coordinates in pixel values (doubles): x y z values for each point (single for sphere, two for cylinder, cone and parallelepiped and four for tetrahedron), plus eventually radius (for sphere, cylinder and cone), or more complex entries (see below) for tetrahedral mesh or Gwyddion height field.
- material type (0: standard material, 1: tabulated material, 2: Drude model (not recommended), 3: CP3 model (not recommended), 4: CP model via Recursive Convolution method, 5: CP model via Auxiliary Differential Equations method, 6: CP model via Piecewise Linear Recursive Convolution method, 10: perfect electric conductor, 99: data from [optical database](#)) followed by:
  - relative permittivity, relative permeability, electric and magnetic conductivity as double values for material type=0, and 1 (both representing linear material)
  - epsilon, omega\_p and nu for type=2 (Drude model)
  - epsilon, sigma and three sets of a, phi, omega and gamma for type=3 (CP3, in development)
  - epsilon, omega, gamma and two sets of a, phi, omega and Gamma for type=4 (CP)
  - epsilon, static sigma, omega, gamma and two sets of a, phi, omega and Gamma for type=5 and 6 (ADE and PLRC approach for CP model) (*Bug in documentation fixed!*)
  - nothing for material type=10 (PEC)
  - [material name](#) for material type=99, e.g. Al2O3

so the entry looks for example as (4 100 100 100 20.5 0 22.13 1 0 0) for sphere with radius 20.5 pixels, position (100, 100, 100) and relative permittivity of 22.13 (rest or material properties is same as for vacuum). Material file for two dielectric nonabsorbing spheres and single absorbing parallelepiped can therefore look like:

```
4 50 100 100 20.5 0 22.13 1 0 0
4 150 100 100 20.5 0 22.13 1 0 0
8 30 30 160 170 170 170 0 20 1 2000 0
```

Note that the material data are interpreted succesively, overwriting previous values in the computational volume if there is an intersection, so you can create relatively complex geometries. Also, if there is MEDIUM\_LINEAR, directive as well in the parameter file, this is performed before MEDIUM\_VECTOR data interpretation (so vector data can overwrite them).

See Example 2 for more details of material parameters use.

For metals, CP model is at present the most suitable approach implemented in GSvit. CP model (in fact Drude + 2 critical points model) is based on this work: *A. Vial, T. Laroche, Appl Phys B (2008) 93: 139-143*, giving the following values for different materials (here already in GSvit material file format including material type (4)):

```
4 15.833 1.3861e16 4.5841e13 1.0171 -0.93935 6.6327e15 1.6666e15 15.797
1.8087 9.2726e17 2.3716e17 (silver)
4 1.1431 1.3202e16 1.0805e14 0.26698 -1.2371 3.8711e15 4.4642e14 3.0834
-1.0968 4.1684e15 2.3555e15 (gold)
4 1.0000 2.0598e16 2.2876e14 5.2306 -0.51202 2.2694e15 3.2867e14 5.2704
0.42503 2.4668e15 1.7731e15 (aluminium)
4 1.1297 8.8128e15 3.8828e14 33.086 -0.25722 1.7398e15 1.6329e15 1.6592
0.83533 3.7925e15 7.3567e14 (chromium)
```

Alternatively the same dispersion model can be solved using two other techniques, Auxiliary Differential Equations and Piecewise Linear Recursive Convolution, whose implementation is both based on *K. Chun, H. Kim, H. Kim, Y Chung, PIERS 135, 373-390, 2013*

. In the formulas there is a static conductivity term in addition, which is by many authors treated as zero (absorption is handled by imaginary part of permittivity through the model anyway). The implementation in GSvit was tested with zero conductivity, giving same reflectivity for flat metal as tabulated values (and same as for Recursive Convolution technique).

In original article by Chun et al. the folloing metals were fitted (presented already with material type and zero conductivity formatted for GSvit use with ADE approach) (*Bug in documentation fixed!*):

```
5 0.89583 0 13.8737e15 0.0207332e15 1.3735 -0.504659 7.59914e15 4.28431e15
0.304478 -1.48944 6.15009e15 0.659262e15 (silver)
5 1.11683 0 13.1839e15 0.109173e15 3.04155 -1.09115 4.20737e15 2.35409e15
0.273221 -1.18299 3.88123e15 0.452005e15 (gold)
5 1.82307 0 13.3846e15 0.163439e15 2.57278 -1.56922e-8 6.65296e15 3.80643e15
0.638294 -1.22019 3.39199e15 0.472389e15 (copper)
```

If **tetrahedral mesh** is provided in [Tetgen .node and .ele format](#), the following parameters are given after entity type (preceding material type and material parameters):

```
filebase attribute_number material_index xshift yshift zshift xmult ymult
zmult
```

Parameter `filebase` determines the filename of `.node` and `.ele` files (`filebase.node`, `filebase.ele`) that are defining the set of tetrahedrons. Attribute `_number` is used to set which attribute of the `.node` and `.ele` file will be used to assign the appropriate material. Loaded node positions are multiplied by `xmult`, `ymult`, `zmult` values and then shifted by `xshift`, `yshift`, `zshift` vector. This can be used to move and scale your data into computation mesh.

If there are no attributes in the `.ele` file, or there are but `attribute_number` is -1, all the tetrahedrons will be treated as the material. If `attribute_number` is zero or positive and there are attributes in the `.ele` file, `material_index` defines the subset of tetrahedrons (with the same index as the appropriate attribute) that will be used as material. Using several lines in your vector material definition file using the same `filebase` you can assign different materials to your set of tetrahedrons.

As an example a vector material file entry could be following for a cube given by tetrahedral mesh with no attributes (note that no attributes means no need for attribute number selection), no shift and no scaling of the mesh (mesh is intended for 200x200x200 voxels volume):

```
21 cube.1 0 0 0 0 0 1 1 1 0 5 1 0 0
```

Corresponding node file (`cube.1.node`) would look like this (indentation is not relevant, lines starting with '#' sign before and after header are skipped):

```
# my little cube
8 3 0 0
# node list
1 50 50 50
2 151 50 50
3 151 151 50
4 50 151 50
5 50 50 151
6 151 50 151
7 151 151 151
8 50 151 151
```

Corresponding element file (`cube.1.ele`) would look like this:

```
# my little cube
6 4 0
# elements (tetrahedrons), links to corresponding node list
#
1 6 7 1 5
2 1 8 3 4
3 3 7 1 2
4 1 7 6 2
5 1 7 3 8
6 7 8 1 5
```

If a piece of mesh should not be used, or different materials should be assigned to different parts of the mesh, use attributes in `.ele` file as follows:

```
21 cube.1 0 1 0 0 0 1 1 1 0 4 1 0 0
21 cube.1 0 0 0 0 0 1 1 1 0 5 1 0 0
```

Here we expect that tetrahedrons have at least single attribute and this attribute (attribute 0) is used for detection of material. Corresponding element file (cube.1.ele) would now look like this:

```
# my little cube
6 4 1
# elements (tetrahedrons), links to corresponding node list
#
1      6      7      1      5      1
2      1      8      3      4      0
3      3      7      1      2      1
4      1      7      6      2      0
5      1      7      3      8      1
6      7      8      1      5      0
```

If **Gwyddion height field** is provided in [Gwyddion](#) format, the following parameters are given after entity type (preceding material type and material parameters):

```
filename channel mask i j k xoffset yoffset zoffset depth
```

Parameter filename corresponds to .gwy file that will be loaded (corresponding channel - if you have only one height field in your file and you haven't done some complex data processing it is probably the channel 0). If parameter mask is 1, only data under mask are used for this purposes (see Gwyddion documentation to see what a mask is). If parameter mask is -1, the inverse of mask is used. Note that real Gwyddion datafield dimensions are used to scale the datafield within the computational space. Vector (i j k) in voxel coordinates defines the relative coordinate center in computation space and direction. (e.g. -1 -1 10 means that the field will be oriented in z normal and its zero coordinate will be shifted by 10 voxels in z). Parameters xoffset, yoffset and zoffset are in dfield physical coordinates and are used to further shift the dfield if necessary. If these are zero, top left corner is aligned. Parameter depth (in voxels) defines the depth to which the material is assigned (with same orientation as the axis).

As an example, the vector material file can look like this for use of channel 2, y axis normal orientation (zero at voxel 50), inverse of mask used, depth 30 voxels and a slight shift in xy direction:

```
22 grating.gwy 2 -1 -1 50 -1 1e-7 1e-7 0 30 0 5 1 0 0
```

Here the computational volume was 200x200x200 voxels and data field had physical dimensions larger than computational volume.

## BOUNDARY\_ALL

type

Set boundary condition of whole volume to a given type:

- **none** which means no boundary treatment providing reflection similar to perfect electric conductor,
- **liao** which means 2nd order absorbing (Liao) providing quite good absorption but not such good as the CPML boundary condition
- **cpml** which means convolutional perfectly matched layer (CPML) with parameters:

depth  
power  
sigma\_max  
a\_max  
kappa\_max

where sigma\_max, alpha and kappa\_max are used to generate coordinate stretching and damping scaled by polynom of power on CPML region of thickness given by depth. If sigma\_max is set as -1, it will be automatically calculated as the optimum value (given by CPML power, grid spacing and free space impedance).

For computation to be stable, sigma\_max and alpha must be positive and kappa\_max must be greater than one. If kappa\_max=1 algorithm is equal to conventional PML and no coordinate stretching is performed

As an example, to construct a 10 cells thick CPML region with polynomial scaling with power of 3 and automatically set optimum sigma\_max value use

```
BOUNDARY_ALL cpl
10 3 -1 0.03 4
```

## **BOUNDARY\_X0/BOUNDARY\_XN/BOUNDARY\_Y0/BOUNDARY\_YN/BOUNDARY\_Z0/BOUNDARY\_ZN**

*type*

Set boundary condition of a given boundary to a given type (types are same as for BOUNDARY\_ALL). Some combinations may lead to instabilities, e.g. corner of cpl and liao region.

## **MBOUNDARY\_X0/MBOUNDARY\_XN/MBOUNDARY\_Y0/MBOUNDARY\_YN/MBOUNDARY\_Z0/MBOUNDARY\_ZN**

*type position*

Artificial boundary inside material, now only periodic one is supported. Position is in pixel coordinates. All unset values are set to computational volume boundaries. Only periodic boundary condition is supported now. To create periodic boundary condition in x direction ranging from pixel coordinates 10 to 50, you need to set:

```
MBOUNDARY_X0
periodic 10
```

```
MBOUNDARY_XN
periodic 50
```

Note that periodic boundary condition for total/scattered field formalism incident wave for angles different from main axes of computational volume is not supported.

## **Medium modifiers**

### **MEDIUM\_GROW**

*i0 j0 k0 in jn kn mat\_index add\_index subsampling nparticles jump\_mobility jump\_probability random\_seed*

Simulates growth of tabulated material of given index (parameter add\_index) on material with given



index (parameter `mat_index`). Growth is realized by ballistic deposition using random particle flight and its attachment that can be followed by some relaxation. Simulation is performed within box defined by (`i0 j0 k0` in `jn kn`) that can be eventually subsampled (parameter `subsampling`) to get better control over results. Particles are flying from box boundaries in random direction unless they leave box or get attached to the material. Materials that are not listed in this directive have no impact on the process (as they would be vacuum). Jump mobility is given in voxel units and controls maximum distance allowed for relaxation, jump probability controls probability of such process (in range of 0-1). Number of particles is typically in range of tens of thousands at least. Random seed can be any integer to get same result or -1 to generate seed automatically. As an example to grow material of index=2 (second entry in material file) on material of index=1 (first entry in material file, with `subsampling=2` you can do the following:

#### **MEDIUM\_GROW**

```
20 20 20 280 280 280 1 2 2 250e6 4 0.8 1
```

Note that for high subsampling the process can be slow and memory demanding. Also note that to add material to the material file without adding any real object (e.g. if you want to grow something that is nowhere else in your computational geometry) you can add a parallelepiped of zero dimensions.

*Note that this option is not supported for direct editing by XSvit in this version*

#### **MEDIUM\_ROUGHEN**

*radius\_peak radius\_span iterations probability material\_index void\_index random\_seed*

Adds roughness to objects consisting of defined tabulated material (parameter `material_index`) adding this material and void or any other material (parameter `void_index`) to the object randomly.

Roughness is controlled by parameter `radius_peak` and `radius_span` (both in voxel coordinates) that control radius and dispersion of spheres that are added. Parameter `probability` controls amount of spheres added in every point. Random seed can be any integer to get same result or -1 to generate seed automatically. Note that materials (parameter `material index`) are counted from 1 as they are loaded from vector material file (so the first material listed there has index of 1). Material with `index=0` is vacuum by default. As an example, to add roughness to a sphere (the only object in material file), using 20 iterations of adding and removing spheres of radius  $5 \pm 2$  voxels, add this:

#### **MEDIUM\_ROUGHEN**

```
5 2 20 0.01 1 0 1
```

*Note that this option is not supported for direct editing by XSvit in this version*

#### **MEDIUM\_SPECTRAL**

*sigma T material\_index random\_seed*

Adds roughness to objects consisting of all tabulated materials (parameter `material_index` is only reserved for future use) using spectral synthesis and vector displacement method. Roughness parameters `sigma` and `T` controlling variance and correlation length are given in voxels. Random seed can be -1 to get it randomly.

#### **MEDIUM\_EXPRESSION**

*i\_start j\_start k\_start i\_end j\_end k\_end material\_index void\_index max\_distance distance\_mode expression*

Alters object boundary using some analytical expression. In the expression, `x`, `y` and `z` mean the voxel coordinates. Basic mathematical functions and constants (`pi`) can be used. As an example, this combination of sine functions can create quite chaotic surface shape:

**MEDIUM\_EXPRESSION**

10 10 10 290 290 290 1 0 10 1

$0.5 + 0.08 \cdot \sin(x/2) + 0.08 \cdot \sin(y/3) + 0.08 \cdot \sin(z/3.8) + 0.08 \cdot \sin((x+y)/5) + 0.08 \cdot \sin((y+z)/2.5) + 0.08 \cdot \sin((x+z)/4.2)$

**MEDIUM\_SMOOTH**

*unused\_integer\_parameter*

Performs smoothing vector material. Smoothing means locally averaging the optical constants (e.g. permittivity). This is a very simple way how to reduce staircasing effects. However it is physically reasonable only in some cases (recalling e.g. effective medium approximation). For metals the procedure is under development and is not recommended for use in present version and for PEC it cannot be applied at all.

**Field sources****SOURCE\_POINT**

*i j k mode (filename, values)*

Point source at position (i j k) using electric and magnetic field intensity time dependence described in file filename (mode=0) or generating such file for sine or pulsed sine waveform. If a text file is used, it consists of integer determining total number of values and successive sets of values consisting of (step, ex, ey, ez, hx, hy, hz). For "mode=1" the source file is automatically generated (file "tmpsource" in the current directory) providing a sine wave source; the parameter after "mode" is therefore wavelength in meters followed by electric field amplitude. Finally, two parameters theta and phi determine the source orientation. For "mode=2" the same happens for sine wave damped by a gaussian envelope, parameter "mode" is therefore followed by wavelength and by gaussian envelope width, given in integer steps of the simulation (e.g. 20), and then electric field amplitude. Again, at the end, two parameters theta and phi determine the source orientation. Theta and phi equal to zero correspond to x-direction electric field point source.

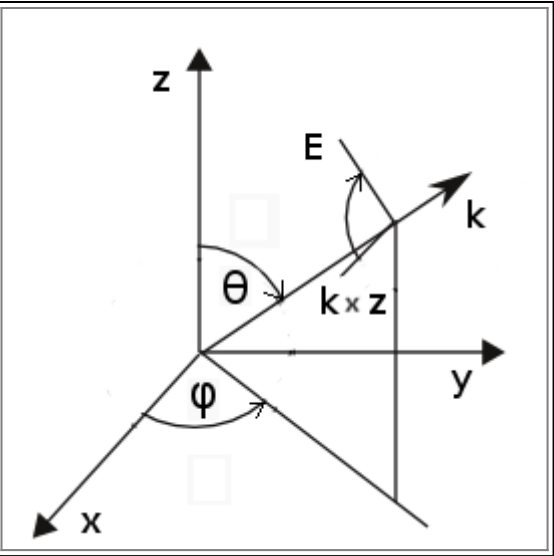
**SOURCE\_TSF**

*i\_start j\_start k\_start i\_end j\_end k\_end theta phi psi mode (filename, values)*

Plane wave source using total/scattered field formulation. Six integers determine volume that is used for field propagation, theta and phi determine wave direction and psi its polarisation. Parameter "mode" distincts different source definition. For "mode=0" a filename is provided pointing to a text file containing number of values N followed by N pairs of values step number - electric field value. N needs to be at least the total number of steps in simulation. For "mode=1" the source file is automatically generated (file "tmpsource" in the current directory) providing a sine wave source; the parameter after "mode" is therefore wavelength in meters followed by electric field amplitude. For "mode=2" the same happens for sine wave damped by a gaussian envelope, parameter "mode" is therefore followed by wavelength and by gaussian envelope width, given in integer steps of the simulation (e.g. 20), and then electric field amplitude.

Note that in present version the TSF source is in vacuum, material cannot cross it.

Orientation of axes of incoming wave is shown in the following image, table shows some typical useful values of parameters:

direction	polarisation	theta [deg]	phi [deg]	psi [deg]	
x axis	y	90	0	0	
x axis	z	90	0	90	
y axis	x	90	90	0	
y axis	z	90	90	90	
z axis	x	0	0	90	
z axis	y	0	0	0	

See Example 2 for details of use.

**TSF\_SKIP** *boundary*

Specifies boundary that should be excluded from TSF application. Parameter "boundary" is string denoting which boundary is being set (i0, j0, k0, in, jn, kn, depth N). Note that in principle TSF should be applied on all the boundaries to work properly, but in case of special materials or boundary conditions some boundary skipping can make sense. The special boundary setting "depth" followed by a positive integer number, e.g. "depth 5" causes solver to skip the TSF application in all the places with some material (not vacuum) and even some number of voxels (parameter depth) close to it. This is useful to remove only some area where material is traversing the TSF boundary from the TSF application.

**TSF\_GAUSSIAN\_Z**

*i\_center j\_center i\_radius j\_radius*

Enable Gaussian multiplier of the TSF input data providing a Gaussian beam. Working only for TSF source oriented in z direction and for normal incidence. Beam is centered in i\_center, j\_center position and has width settable to each direction independently i\_radius, j\_radius. Everything is in voxel coordinates.

**SOURCE\_LTSF**

*i\_start j\_start k\_start i\_end j\_end k\_end theta phi psi n\_materials mat1\_pos mat1\_epsilon mat1\_mu mat1\_sigma mat\_sigast .... mode (filename, values)*

Plane wave source using layered total/scattered field formulation as published by I.R. Capoglu, G.S. Smith: IEEE Transactions on Antennas and Propagation 02/2008, 56:1. In contrast to SOURCE\_TSF, here the material can be formed by N layers in z-direction (in present implementation only dielectric and non-absorbing). Incident wave however can cross the sample at angle as well. Layers need to be introduced both in parameters of the source and in material description files (as set MEDIUM\_LINEAR or MEDIUM\_VECTOR) and the values of material parameters need to match at LTSF boundary. First six integers determine volume that is used for field propagation, theta and phi determine wave direction and psi its polarisation. This is followed by number of interfaces. For every interface its position in z direction and four material parameters are entered. By default the zero interface starts at z=0 and has permittivity of vacuum, so it does not need to be entered. Plane wave should start at vacuum. In order to create single free standing film we therefore need to enter two interfaces, upper and lower as seen in the example below. Next parameter, "mode", distincts again different source definition (same as for TSF). For "mode=0" a filename is provided pointing to a text file containing number of values N followed by N pairs of values step number - electric field value. N needs to be at

least the total number of steps in simulation. For "mode=1" the source file is automatically generated (file "tmpsource" in the current directory) providing a sine wave source; the parameter after "mode" is therefore wavelength in meters followed by electric field amplitude. For "mode=2" the same happens for sine wave damped by a gaussian envelope, parameter "mode" is therefore followed by wavelength and by gaussian envelope width, given in integer steps of the simulation (e.g. 20), and then electric field amplitude.

As an example to create a plane wave (with a pulse time dependency and polarisation angle 0.3 rad) incident at angle on a free standing dielectric layer (in 200x200x200 voxels computational volume), use the following: SOURCE\_LTSF 30 30 30 170 170 170 0.3 0.3 0.3 2 80 3 1 0 0 120 1 1 0 0 2 2e-7 50 5

Note that in this case the material parameters need to match the source, so e.g. using MEDIUM\_VECTOR definition we can use this material file:

8 20 20 80 180 180 120 0 3 1 0 0

## LTSF\_GAUSSIAN

*i\_center j\_center i\_radius j\_radius*

Enable Gaussian multiplier of the LTSF input data providing a Gaussian beam. Now working only for normal incidence. Beam is centered in *i\_center*, *j\_center* position and has width settable to each direction independently *i\_radius*, *j\_radius*. Everything is in voxel coordinates.

## SOURCE\_SF

*theta phi psi mode (filename, values)*

Plane wave source using pure scattered field formulation, working only for PEC interfaces. The parameters for source direction and data definition are the same as for TSF source. Note that SF source is not supported by GPU in present version.

See Example 3 for details of use.

## SOURCE\_TSFF

*i\_start j\_start k\_start i\_end j\_end k\_end thetamax fdist polarisation n m mode (filename, values)*

Z direction oriented focused wave source using total/scattered field formulation with multiple plane waves decomposition according to algorithm published in *I.R.Capoglu, A. Taflov, V. Backman, Optics Express 23 (2008) 19208*. Six integers determine volume that is used for field propagation, thetamax determines maximal angle of incoming light, fdist the focal distance in voxel units. Polarisation angle of the incoming wave can be controlled by the following parameter. Integer parameters *n* and *m* determine number of plane waves to be integrated (more is better, values around 12, 36 should be already enough). Similarly to plane wave source, parameter "mode" distincts different source definition. For "mode=0" a filename is provided pointing to a text file containing number of values *N* followed by *N* pairs of values step number - electric field value. *N* needs to be at least the total number of steps in simulation. For "mode=1" the source file is automatically generated (file "tmpsource" in the current directory) providing a sine wave source; the parameter after "mode" is therefore wavelength in meters, followed by electric field amplitude. For "mode=2" the same happens for sine wave damped by a gaussian envelope, parameter "mode" is therefore followed by wavelength and by gaussian envelope width, given in integer steps of the simulation (e.g. 20), and finally electric field amplitude.

## SOURCE\_LTSFF

*i\_start j\_start k\_start i\_end j\_end k\_end thetamax fdist polarisation n m n\_materials mat1\_pos mat1\_epsilon mat1\_mu mat1\_sigma mat\_sigast .... mode (filename, values)*

Similar focused source to SOURCE\_TSFF, however now dielectric material layers arranged in *z* direction can be crossed, similarly to SOURCE\_LTSF. Note that in contrast to SOURCE\_TSFF much

more memory is needed for precomputation of the incident field and in present version you can easily run out of memory for larger systems or larger number of computation steps.

### SOURCE\_EXT

*ipos jpos kpos ijstart jkstart ext\_xres ext\_yres ext\_ifrom ext\_jfrom ext\_ito ext\_jto shift filebase\_ex filebase\_ey filebase\_ez filebase\_hx filebase\_hy filebase\_hz*

Uses set of external arrays to inject a source via TSF-like approach. Direction of the source is controlled by ipos, jpos and kpos where only one of these three parameters should be not -1 similarly to image output. Parameters ijstart and jkstart control placement of upper left corner of injected source plane. Parameters ext\_xres and ext\_yres control resolution of the data in external source files and parameters ext\_ifrom, ext\_jfrom ext\_ito and ext\_jto control size and position of the part of external field that is used. Parameters filebase describe naming of source files (so for filebase\_ex="ex" this will be ex\_0000, ex\_0001 for steps 0 and 1). The format of these files corresponds to what we get by OUT\_PLANE directive in ASCII mode. *Note that this directive is experimental, might be unstable and its syntax might change.*

*Note that this option is not supported for direct editing by XSvit in this version*

### SOURCE\_WAVELENGTH

*min center max*

Override automatic wavelength detection mechanism for sources. These (or automatically detected) values are used when listed material (e.g. silica) is used to pick the optical properties at right wavelength from the predefined values. Center value is used for materials that are predefined as lookup table, min and max values are used for materials where we have some dispersion model available.

### Output

Note that in present version every output needs GPU data to be synchronized with CPU, which can take significant time. For really fast simulations try to reduce frequency of data outputs.

### OUT\_FILE

*filename.gwy*

Set filename that will be used for outputting data. Gwyddion file (\*.gwy) holds all data cross-sections (2d data).

### OUT\_POINT

*Ex/Ey/Ez/Hx/Hy/Hz/All nskip i j k filename*

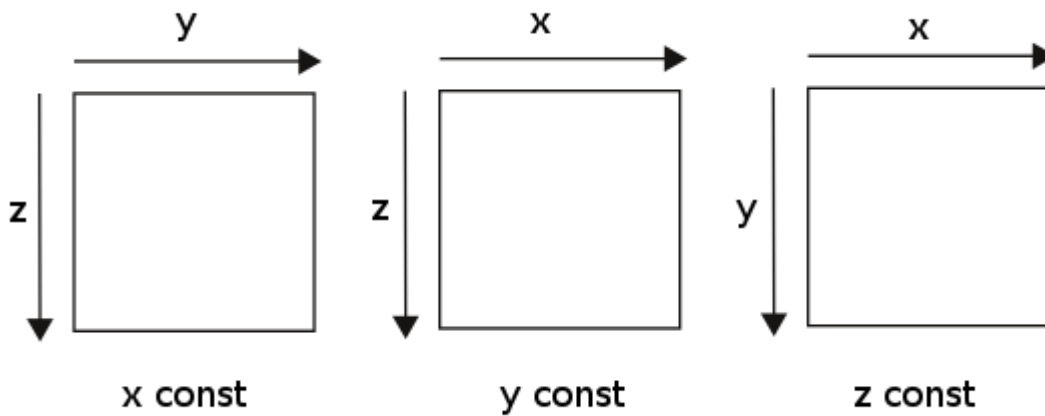
Output values of given component of electric/magnetic field into text file (filename).

### OUT\_IMAGE

*Ex/Ey/Ez/Hx/Hy/Hz/All/Epsilon/Sigma/Mu/Sigast/Material nskip i j k description*

Output image of plane cross-section. Which plane is used is determined by indices i j k; two of them must be -1. All results are saved to a .gwy file, skipping given number of steps (e.g. not outputting image in every step unless nskip=1). Description is a string shown for the channel in Gwyddion data browser.

Note that Gwyddion shows data with top-left corner being center of coordinates, orientation of axes on what is seen in Gwyddion is show below



## OUT\_SUM

*component skip i\_start j\_start k\_start i\_end j\_end k\_end epsilon mu sigma sigma\* filename*

Output sum of electric field intensity (components: ex, ey, ez, all) or absorption (component: abs) extracted from bounding box and material with given properties (epsilon only used for this). If epsilon is -1, no control of this parameter is done and whole box is used. Parameter "skip" controls frequency of file output only (and sync with GPU eventually), values are calculated at each time step anyway and will be output for intermediate steps as well. At present this is tested only on CPU.

## OUT\_SUMTAB

*component skip i\_start j\_start k\_start i\_end j\_end k\_end material filename*

Output sum of electric field intensity (components: ex, ey, ez, all) or absorption (component: abs) extracted from bounding box and material with given properties (nk tabulated values from optical spectra database). Parameter "skip" controls frequency of file output only (and sync with GPU eventually), values are calculated at each time step anyway and will be output for intermediate steps as well. At present this is tested only on CPU.

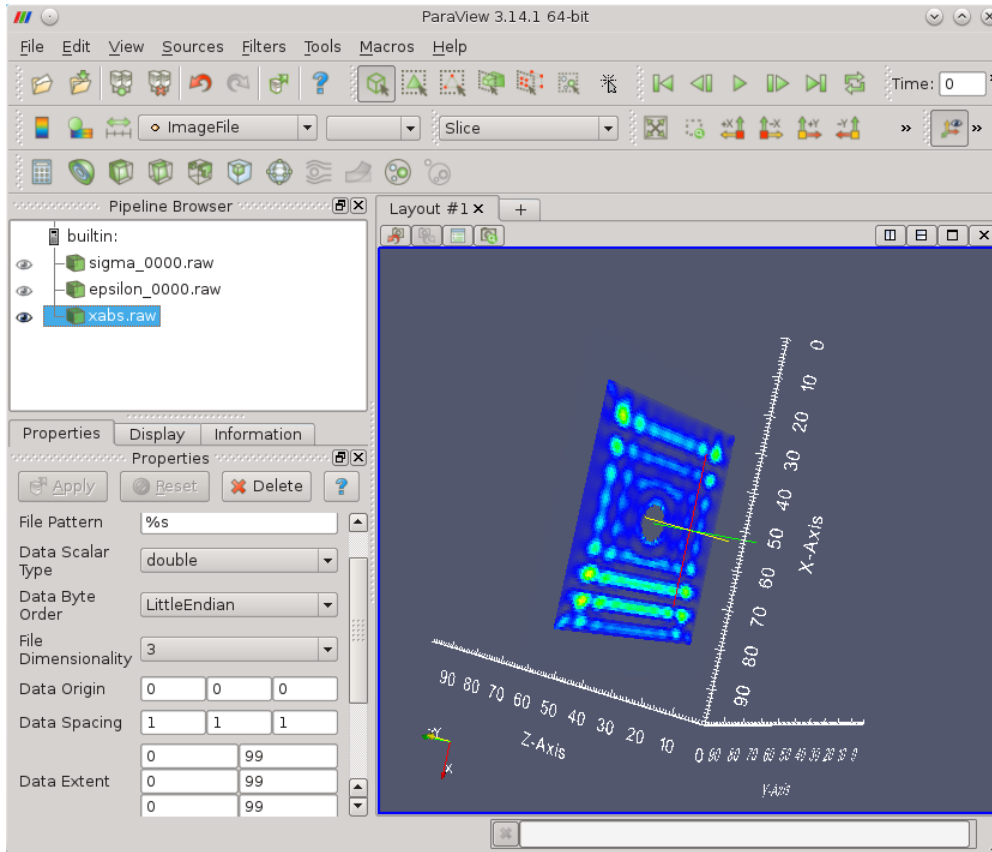
## OUT\_VOLUME

*Ex/Ey/Ez/Hx/Hy/Hz/All/Epsilon/Sigma/Mu/Sigast/Material/Matmode/Abs skip start stop ascii filename*

Output values of given component of electric/magnetic field or material parameters into binary or text file. Whole computational volume is output. Output starts in "start" step and stops before "stop" step. If "Abs" component is requested (meaning local absorption), output in every output step is a sum of the present and all the previous outputs (values in between outputs are not used; this means that to sum absorption from step 100 to 110 you need to run at least 110 computation steps with volume output skip=1 and volume output start=100, stop=110).

If ASCII file (ascii=1) is output, it has following structure: xres yres zres channel (and all the data as an array of values separated by space or end of line).

In binary mode the header is omitted, so only arrays are output, all the array values are doubles (eight bytes), there are no separators. You can read binary output directly by e.g. [Paraview](#) as shown below where a slice of absorption volume of 100x100x100 voxels is visualised (here you can check also data loading parameters for Paraview).



## OUT\_FORCE

*skip i\_start j\_start k\_start i\_end j\_end k\_end filename*

Output optical force acting on volume defined by six integers. X, y, and z component time dependence is output together with its values averaged over source period (source frequency is determined using FFT). Optical force is calculated using Maxwell stress tensor. No media should cross the boundary and scatererr to be evaluated should be placed inside the evaluation volume.

**NFFF** *i0 j0 k0 i1 j1 k1 sum\_from sum\_to*

Near-to far field calculation boundary definition. Needs to be within the computational volume. Parameters i0..k1 define the boundary position, sum\_from and sum\_to define the range of NFFF data summation when applied (not supported now). See example 3 for details of use.

**NFFF\_SKIP** *boundary i\_min/j\_min j\_min/k\_min i\_max/j\_max j\_max/k\_max*

Specifies area that should be excluded from NFFF calculation. Parameter "boundary" is string denoting which boundary is being set (i0, j0, k0, in, jn, kn), the next four numbers describe "upper left" corner and "bottom right" corner of the skipped area. Multiple calls of NFFF\_SKIP can be used to exclude more areas on different boundaries, however at present only one area on each boundary can be set. Note that in principle NFFF should be applied on all the boundaries to work properly, but in case of special materials or boundary conditions some boundary or boundary area skipping can make sense.

**NFFF\_RAMAH\_POINT** *i j k filename*

Far field point designed for time values of electric field output. Can be outside of the computational volume even if it is entered in integer values representing position in computational volume (therefore values can be e.g. negative). See example 3 for details of use.

**NFFF\_SPHERICAL\_AREA** *theta\_res phi\_res radius theta\_from phi\_from theta\_to phi\_to savefile*

Creates set of far field points designed for time values of electric field output. Set of (theta\_res x phi\_res) points are on a sphere of given radius (int integer i.e. voxel units), theta is declination and

phi is azimuth. Parameter savefile determines whether to save all the farfield point dependencies or just put the total output into general output file (in Gwyddion format). As an example, considering a surface with normal oriented in z direction (negative), to cover whole half-sphere above sample for reflection scattering simulation by set of 20x20 points on sphere with radius of 1000 voxels, and not to save intermediate files, write

```
NFFF_SPHERICAL_AREA 20 20 1000 90 0 180 360 0
```

*Note that this option is not supported for direct editing by XSvit in this version, however it can be still visualised.*

#### **NFFF\_PLANAR\_AREA** *ares bres afrom bfrom ato bto orientation distance savefile*

Creates set of far field points designed for time values of electric field output. Set of (a x b) points are on a plane oriented with normal to direction in x, y or z (depending on "orientation parameter" ranging from 0 (x) to 2 (z)). Distance from computation center can be set, in integer i.e. voxel units. Plane offset in "a" and "b" direction and its span (that does not need to match voxel spacing) can be controlled by parameters "afrom", "bfrom", "ato", "bto". Parameter savefile determines whether to save all the farfield point dependencies or just put the total output into general output file (in Gwyddion format).

*Note that this option is not supported for direct editing by XSvit in this version, however it can be still visualised.*

#### **PERIODIC\_NFFF** *i0 j0 k0 i1 j1 k1 per\_ifrom per\_jfrom per\_ito per\_jto*

Periodic near-to far field calculation boundary definition. Suitable namely for use with periodic boundary conditions of same dimensions. Uses only z planes (given by integer k0, k1) but repeats it as many times as given by integer span (per\_ifrom, per\_jfrom, per\_ito, per\_jto). Using periodic repeating values 0 0 1 1 gives the same result as conventional NFFF with skipped all the boundaries except single z plane. Values of periodic repeating can be negative, so e.g. values -1 -1 2 2 will produce result of 3x3 copies of calculated fields centered at the originally computed one.

#### **PERIODIC\_NFFF\_SKIP** *boundary i\_min/j\_min i\_max/j\_max*

Specifies area that should be excluded from periodic NFFF calculation. Parameter "boundary" is string denoting which boundary is being set (k0 or kn as no other boundaries are used in periodic NFFF), the next four numbers describe "upper left" corner and "bottom right" corner of the skipped area. Note that in principle NFFF should be applied on all the boundaries to work properly, but in case of special materials or boundary conditions some boundary or boundary area skipping can make sense.

#### **PERIODIC\_NFFF\_POSTPROCESS** *yes/no start*

Speedup of perodic NFFF by accumulation of the boundary values during computation followed by their processing at the end. First parameter requests the algorithm (0 by default not use it, 1 to use it), second parameter can be used to reduce memory needs skipping integration at beginning of the computation when field is not developed enough anyway. Still can be very memory demaning for longer calculations.

#### **PERIODIC\_NFFF\_RAMAH\_POINT** *i j k filename*

Far field point designed for time values of electric field output in periodic NFFF. Can be outside of the computational volume even if it is entered in integer values representing position in computational volume (therefore values can be e.g. negative).

#### **PERIODIC\_NFFF\_SPHERICAL\_AREA** *theta\_res phi\_res radius theta\_from phi\_from theta\_to phi\_to savefile*



Creates set of far field points designed for time values of electric field output using periodic NFFF. Set of (theta\_res x phi\_res) points are on a sphere of given radius (int integer i.e. voxel units), theta is declination and phi is azimuth. Parameter savefile determines whether to save all the farfield point dependencies or just put the total output power into general output file (in Gwyddion format). As an example, considering a surface with normal oriented in z direction (negative), to cover whole half-sphere above sample for reflection scattering simulation by set of 20x20 points on sphere with radius of 1000 voxels, and not to save intermediate files, write

```
PERIODIC_NFFF_SPHERICAL_AREA
20 20 1000 90 0 180 360 0
```

*Note that this option is not supported for direct editing by XSvit in this version, however it can be still visualised.*

## Graphics card use

### GPU

*ngpus*

Set number of graphics cards to be used (indexed as CUDA indexes them). If this command is not used or set to zero, calculation is performed on PC processor. See example 1 for details of use. Note that at present version use of multiple GPUs together is implemented, but untested.

### UGPU

*number*

Set GPU with given index to be used for calculations (indexed as CUDA indexes them). This can be used for example to run several different calculations on different cards. See example 1 for details of use.

### GPU\_QUERY

*0/1*

Search for available GPUs, detecting and printing their capabilities prior to using any of them (default 1, which means true). Skipping this step can prevent large delays on some supercomputing systems with very large number of boards and PCI buses, however it is not necessary nor recommended for use on a standard PC.

## General commands

### VERBOSE

*0-4*

Set text output (step by step), from full (4) to silent mode (0).

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