Simulator of light propagation in composites (SOLPIC)

User manual

Table of Contents

System requirements

SOLPIC general system requirements are Linux/Unix machines with gfortran installed. Any text editor (vi, gimp etc.) will be suitable to edit the input files.

Warranty

The SOLPIC comes with no absolutely warranty. Authors are not responsible to whatever damage, including damage to scientific reputation, this program might cause. Efforts were made to make the program stable. However, it is definitely possible to choose a set of parameters for which the program will give wrong results, senseless results, or simply crash. Treat this program not as a fool-proof product, but more as an experimental setup, which can give all kinds of results depending on handling.

License agreement

The SOLPIC can be used in any way (including modification of the program) for any needs of the members of ATLANTIC RISE project consortium.

Setup

1. Unzip the installation archive (tar -xf solpic.tar) in your working directory.
2. Make the file compile.sh executable (chmod 770 compile.sh).
3. Run the compile.sh (./compile.sh). Several runs may be required. Ignore the warnings. Check that the executable file a.out has been created.
4. To run the program, run a.out (./a.out).

Input and output files

Input files are:

input.dat, input_pulses.dat, disp_host.dat, disp_host.f, disp_incl.dat, disp_incl.f, freq.dat, dip_mom.dat

Output files are: field_N.dat and sp_N.dat, where N runs from 1 to 10.

The files are described in what follows.

input.dat

File input.dat must contain 24 lines which define various parameters related to simulation. All the parameters must be set, there are no default values. Including less than 24 lines will produce an error; including more than 24 lines will lead to excess lines being ignored.

Each of the lines has the structure

identifier value

,where identifier is a case-sensitive string which describes the parameter being set and value is its value, eihter integer or real. Almost all values, with an exception of the ionization potential, are defined in SI units. The order in which the parameters are set is not important. The parameters can be given using the floating-point notation: 5d-5 means to $5x10^{-5}$

The parameters are described in the following table:

Identifier	Integer/real	Description	Typical value	Units
nz	Integer	Number of steps of propagation along the z coordinate. It is recommended that it is a multiple of 10.	1000	-
dz	Real	Length of a step in z coordinate	1d-6	m
filling_factor	Real	Volume fraction of inclusions	0.01	-
chi2h	Real	Second-order susceptibility of the host medium	0	m/V
chi3h	Real	Third-order susceptibility of the host medium	1d-22	m^2/V^2
chi2i	Real	Second-order susceptibility of the inclusions	0	m/V
chi3i	Real	Third-order susceptibility of the inclusions	1d-22	m^2/V^2
ion_p	Real	Ionization potential of inclusion, ***in electronvolts***. It is assumed that the ioniaztion potential of inclusions is lower than the ionization potential of the host medium.	5	eV
n_pulses	Integer	Number of input pulses	1	-
nt	Integer	Number of grid points in time domain. Preferred to be a power of 2.	65536	-

dt	Real	Grid step in time domain	0.02d-15	s
nlinesdh	Integer	Number of lines in the file disp_host.dat. It can be set to a special values of: 1, indicating to take only the first refractive index and loss values of the disp_host.dat and use it for the whole spectral domain 0, indicating to use the dispersion formula from disp_host.f file to calculate te dispersion. In this case, disp_host.dat is ignored	0	-
nlinesdi	Integer	Number of lines in the file disp_incl.dat. It can be set to a special values of: 1, indicating to take only the first refractive index and loss values of the disp_incl .dat and use it for the whole spectral domain 0, indicating to use the dispersion formula from disp_incl.f file to calculate te dispersion. In this case, disp_incl.dat is ignored	0	-
f_low	Real	Lowest frequency in the spectrum to be included. All frequencies below this will be filtered out at each z step.	0.05d15	s^{-1}
f_high	Real	Highest frequency in the spectrum to be included. All frequencies below this will be filtered out at each z step.	5d15	s^{-1}
ngr	Real	Group refractive index	1.45d0	-
nlev	Integer	Number of excitonic energy levels	2	-
part_c	Real	Particle (molecular or atomic) density in the inclusion material.	3d28	m^{-3}
T1	Real	Population decay time of the excitons	1000d-15	s
T2	Real	Polarization decay time of the excitons	100d-15	s
psize	Real	Radius of the inclusions	1.5d-9	m
nmask	Integer	Number of grip points in time to be masked out at the beginning and end of the time domain at each step. It is recommended to be around 2% of nt.	1000	-
rk_order	Integer	Order of Runge-Kutta method to be used. Can be set to 1, 2, or 4.	4	-
nu	Real	Conduction electron collision rate	0.5d15	s^{-1}

input_pulses.dat

This file contains three lines for each of the input pulses, with number of pulses defined by n_pulses in input.dat. It is recommended to put the strongest pulse first. For each of the pulses, it necessary to

provide the central circular frequency, FWHM duration, as peak intensity, in SI units, at separate lines.

disp_host.dat / disp_incl.dat

Files describe dispersion of host medium and inclusions, correspondingly, and should have at least nlinesdh and nlinesdi lines, respectively. Each line should contain three real values: frequency ω, real part of n(ω), and imaginary part of n(ω). The values of frequencies can be chosen arbitrary, the frequencies do not have to be equidistant, but they should be ordered from the lowest to the highest.

disp_host.f / disp_incl.f

Files describe dispersion of host medium and inclusions, correspondingly, using analytical formulas. Depending on nlinesdh and nlinesdi, either disp_host.dat / disp_incl.dat or disp_host.f / disp_incl.f will be used, as described in the above table. The files should have the following structure:

The files disp_host.f / disp_incl.f should have the following structure:

```
subroutine disp_host_func(f_c,xn_re,xn_im)
implicit double precision (a-h,o-p,r-z)
xn_re=[real part of the refractive index as a function of circular frequency f_c]
xn_im=[imaginary part of the refractive index as a function of circular frequency f_c]
end


subroutine disp_incl_func(f_c,xn_re,xn_im)
implicit double precision (a-h,o-p,r-z)
xn_re=[real part of the refractive index as a function of circular frequency f_c]
xn_im=[imaginary part of the refractive index as a function of circular frequency f_c]
end
```

Note that the calculation can be more complicated than just providing two formulas, the number of lines ad the complexity of the calculations are not limited.

freq.dat

Circular frequencies of the excitonic levels ω_i, in SI units. Number of levels is set in input.dat by n_lev. Order of the frequencies is arbitrary, but it should correspond to the order of the dipole moments in the file dip_mom.dat below. Each value should be provided on a separate line.

dip_mom.dat

Dipole moments d_{ij} of the transitions between the excitonic levels, in SI units (C*m). There must be n_lev^2 values in this file. Order of the levels should correspond to order of the frequencies. The second index is changed first, so for three levels, the order is $d_{11}, d_{12}, d_{13}, d_{21}, d_{22}, \ldots$. Each value should be provided on a separate line.

Output files

field_N.dat

Files field_N.dat contain electric fields, for N=1,2,3,...,10 after 10%,20%,30%,...,100% of the propagation. Each file contains nt lines, each line consists of position of time grip point and electric field at this point. Both values are in SI units.

sp_N.dat

Files sp_N.dat contain squared module of the electric field spectra, for N=1,2,3,...,10 after 10%,20%,30%,...,100% of the propagation. Each file contains nt/2-1 lines, each line consists of circular frequency and spectrum value $|E(\omega)|$ at this frequency. Frequency is in SI units, spectrum values are in arbitrary units.