SIRIS 2

The manual

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About the document

This is the instruction manual for the SIRIS Fortran-77 code developed primarily by Karri Muinonen.

The theoretical background is presented as it appears in the following paper: Karri Muinonen, Timo Nousiainen, Hannakaisa Lindqvist, Olga Muñoz, Gorden Videen, *Light scattering by Gaussian particles with internal inclusions and roughened surfaces using ray optics*; *JQSRT* 110 (2009) 1628–1639.

Purpose

SIRIS is a code for simulating light scattering by Gaussian-random-sphere particles that are large compared to the wavelength of the incident light. The three types of scattering that the code is able to simulate are ray optics, diffraction, and geometric ray optics. The latter utilizes ray optics that, in addition to Fresnelian reflection and refraction, accounts for diffuse scattering. The acronym RODS (Ray Optics with Diffraction and Specular interactions) will be used for this approach.

Three different approaches for diffusely scattering media can be considered:

1) The diffuse scatterers can constitute an *internal medium* spanning uniformly across the particle interior (DIM, for diffuse internal medium), or
2) The scatterers can constitute an *external medium* (DEM, for diffuse external medium) covering the surface of the particle. The layer thickness is small relative to the size of the particle.
3) No diffuse scatterers.

Whereas the former medium is a true three-dimensional medium, the physical thickness of the latter is negligible as compared to the size of the particle, and diffuse scattering occurs within a single infinitesimal location on the surface. For each diffuse scattering process, the full scattering phase matrix is accounted for, as well as the full state of polarization of the incident Stokes vector. The scattering phase matrix can be specified using cubic splines for a user-defined matrix or using an empirical double Henyey–Greenstein matrix with four parameters: the total asymmetry parameter, the forward and backward asymmetries, and the maximum-polarization parameter.

Mathematical formulation

See the original paper that is referred to on the cover page (Muinonen et al. 2009).

Structure and compilation

SIRIS is a Fortran-77 code that currently works only in a single-processor mode. The library includes the following modules and subroutines:

Corrfunc.f   (Correlation functions)
- SGSCFSTD: standard deviations for the spherical harmonics coefficients
- CSELL: correlation length and angle, derivatives
- CSLEGP: Legendre expansion of the correlation function
- CS1CF: power law correlation function
- CS2CF: modified Gaussian correlation function
- CS3CF: input correlation function coefficients from file

Discrets.f   (Particle discretization)
- TRIDS: triangles

Fordif.f   (Forward diffraction)
- DIFFH: averaged Fraunhofer diffraction by circular projections
- DIFUPDATE: updates scattering phase function due to diffraction
- DIFINT: integrand for diffraction computation
- DIFSQG: diffraction phase function, efficiency, and asymmetry parameter
- DIFCS: precomputation of cosines and sines
- DIFIN: input forward diffraction from a file
- DIFOUT: forward diffraction output

Fordifg.f   (Forward diffraction for Gaussian spheres)
- GDIF: main algorithm for forward diffraction

Geoopt.f   (Geometric optics)
- REFREF: specular reflection and refraction
- SCATTER: scattering cross section and phase matrix updates
- ABSORB: absorption cross section update
- MIRROR: mirror reflection law
- SNEL: Snel's law of refraction
- FRESNEL: Fresnel coefficients for reflection and refraction
- MREFREF: Mueller matrix for reflection and refraction
- MROTATION: Mueller matrix for rotation
- MSCATTER: Mueller matrix for scattering
- MPRO: Product of two Mueller matrices
- MIPRO: Product of Mueller matrix and the matrix of Stokes parameters
- RAYINI: initial rays
- RAYPILE: pile of rays
- GEOIN: input geometric optics from a file
- GEOOUT: geometric optics output

Geooptgh.f   (Geometric optics for Gaussian spheres)
- GGEO1:   main algorithm for geometric optics for DIM
- GGEO2:   main algorithm for geometric optics for DEM

Gsg.f   (Gaussian-sphere generator)
- RGSTD: discrete triangle representation
- RGSHULLTD: concave-hull discrete triangle representation
- RGS: radial distance
- SGS: logarithm of radial distance
- SGSCF: spherical harmonics coefficient generation

Insect.f   (Particle-line intersections)
- RTD: radial distance for a triangle-discretized object
- RTDSILH: silhouette and projected area of a triangle-discretized object
- ISTRI: intersection with a triangle-discretized object
- ISTRIE: intersection with a triangle-discretized object (external)
- ISTRIEI: intersection with a triangle-discretized object (external, init.)
- ISPLANE: intersection with a plane

Insectg.f   (Particle-line intersections for Gaussian-spheres)
- RSILH: silhouette and projected area of a non-discretized object

Numint.f   (Numerical integration)
- GAULEG
- SPLINE
- SPLINT

Orient.f   (Particle orientation)
- PRANOR: random orientation using Euler angles

Radtrans.f   (Radiative transfer)
- SCART: scattering process
- ABSORBRT: absorption cross section update in multiple scattering

- PMATRIX: input scattering phase matrix
- PRAYLV: Rayleigh scattering phase matrix
- PHGV: Henyey-Greenstein scattering phase matrix
- PSPLIVI: initialization of spline interpolation for phase matrix
- PSPLIV: spline interpolation for phase matrix
- CSPSPLIV: cosine-random-number map for spline phase function
- CSVRTBIS: bisectioning algorithm for cosine-random-number mapping
- PCDFSPLIV: c.d.f. of spline phase function
- KEPNM: Kepler's equation solved by Newton's method.

Randev.f   (Random deviates)
- RAN2: uniform deviates within (0, 1)
- RANG2: Gaussian deviates with zero mean and unit standard deviation

Ro.f   (Ray optics)
- RAYOUT: ray optics output

Rog.f   (Ray optics for Gaussian spheres)
- GROOUT: joint parameters

Specfunc.f   (Special functions)
- BESJ0A: Bessel function J_0
- BESJ1A: Bessel function J_1
- BESMS: modified spherical Bessel functions multiplied by exponential
- LEGA: associated Legendre functions
- FACTRL: factorial function
- GAMMLN: logarithmic Gamma function
- GAMMQ
- GSER
- GCF

Voper.f   (Vector calculus)
- VROTEU: vector rotation using Euler angles
- VROTEUT: transpose of vector rotation using Euler angles
- VROTX: vector rotation about the x-axis
- VROTY: vector rotation about the y-axis
- VROTZ: vector rotation about the z-axis
- VPRO: vector product
- SPRO: scalar product
- VDIF: vector difference
- VDIFN: normalized vector difference
- VMV: matrix operation on a vector

The compilation works exactly as the compilation of any Fortran code. For example, using gfortran compiler and the executable program name Grayopt.x, the code can be compiled with the following command:

gfortran -o Grayopt.x Grayopt.f

The executable may be moved to another directory with the input files, and run simply by giving the command

./Grayopt.x

The input of SIRIS 2 consists of one file "Grayopt.in" which includes all the model parameters. In addition, if one wishes to use pre-computed scattering matrix that describes the scattering by the diffuse scatterers, one file called "pmatrix.in" will be required. **Note! It is not necessary to use all the parameters in the file for the model.** Different scenarios and the parameters required for them are listed after each parameter and further described below after the complete list of parameters.

The "Grayopt.in" file includes the following parameters:

1. Geometric optics (1), diffraction (2), or ray optics (3).
   (1) Define #30-38
   (2) Define #39-46
   (3) Define #47-50
2. Diffraction: G-spheres (1) or equiv. spheres (2).
   (1) Define 13-18
   (2) Define ??
3. General (1) or concave-hull mode (2).
4. Correlation function (1=power law, 2=Gaussian, 3=file).
   (1) Define #15
   (2) Define #16
5. Diffuse scattering medium (1).
6. Internal (1) or external diffuse scattering medium (2).
   (1) Define #13, #25
   (2) Define #26
7. Scattering matrix: input (1), Rayleigh (2), D-H-G (3).
   (1) Define #20 and #27, see section "User-defined scattering matrix".
   (2) Define ??
   (3) Define #21-24
8. Wavelength (in length units).
9. Refractive index of the medium. *Medium outside the particle.*
10. Refractive index of the particle: real part.
11. Refractive index of the particle: imaginary part.
12. Mean radius of the particle (in length units).
13. Relative radius of external sphere. *Only required in the concave-hull mode.*
14. Relative standard deviation of radius of the particle.
15. Power law index for C_1 correlation.
16. Correlation angle for C_2 autocorrelation.
17. Minimum degree in C_1, C_2, C_3. *Must be > 0.*
18. Maximum degree in C_1, C_2, C_3. *Must be < 256.*
19. Number of triangle rows in an octant. *Particle shape resol., must be < 180.*
20. Diffuse-medium single-scattering albedo. *See the section "Mathematical formulation".*
21. Diffuse-medium asymmetry parameter. *For defining the D-H-G profile*
22. Diffuse-medium forward asymmetry. *For defining the D-H-G profile*
23. Diffuse-medium backward asymmetry. *For defining the D-H-G profile*
24. Diffuse-medium single-scattering maximum polarization. *For the D-H-G.*

25. Internal diffuse-medium mean free path (in length units). *For DIM, see the section "Mathematical formulation"*
26. External plane-parallel-medium optical thickness. *For DEM see the section "Mathematical formulation"*
27. Number of phase matrix angular points. *Input scattering matrix angle resolution (maximum is 360, or 0.5-degree resolution!)*
28. Number of G-L integration points for cosine map. *?? Use 32.*
29. Number of points in random number array. *?? Use 1000.*

For geometric optics (#1 = 1):
30. Maximum chord number in ray tracing. *If Im(m) > 0.05, use 0.*
31. Number of rays. *Divided among the sample particles! Use a large integer value, at least 1,000,000 (unless you are just testing). The DIM requires more rays than DEM for a reliable result.*
32. Number of sample particles. *For inhomogeneous particles, use large value, and for (nearly) spherical particles, use small value.*
33. Number of scattering angle bins. *Output scattering matrix angle resolution*
Output filenames: *(Note! Max. 8 letters!)*
34. Output of input parameters.
35. Output of parameters.
36. Output of phase function and polarization degree.
37. Output of full scattering phase matrix.

For forward diffraction (#1 = 2):
38. Number of sample silhouettes.
39. Number of scattering angles.
40. Number of azimuthal angles for averaging.
41. Polar-angle grid for cross section computation.
42. Azimuthal grid for cross section computation.
Output filenames: *(Note! Max. 8 letters!)*
43. Output of input parameters.
44. Output of parameters.
45. Output of phase function.

For ray optics (#1 = 3):
Output filenames: *(Note! Max. 8 letters!)*
46. Output of input parameters.
47. Output of parameters.
48. Output of phase function and polarization degree.
49. Output of full scattering phase matrix.

For RODS, there are two different diffuse-scattering methods. One accounts for internal inhomogeneities (diffuse internal medium, DIM) with *the single-scattering albedo, extinction mean free-path length, and scattering phase matrix* as additional parameters. The other one accounts for surface roughness (diffuse external medium, DEM) with *the single-scattering albedo, optical thickness, and scattering phase matrix* as additional parameters.

In the case of DIM, the diffuse scatterers are embedded in a homogeneous and isotropic medium described by the complex refractive index. In the case of DEM, the diffuse scatterers constitute a plane-parallel medium on the surface of the Gaussian random sphere, assuming that both the physical thickness of and the mean free-path length in the medium are negligible as compared to the typical radial distance of the Gaussian sphere.

User-defined scattering matrix

One option of SIRIS is to use a user-defined scattering matrix to describe the diffuse scattering. Because the scattering matrix is often computed using another code, the user should be careful with the compatibility of SIRIS and the scattering matrix formulation. Below, there are listed the two rules of thumb for the matrix:
1. The angle resolution should be 0.5-1, no more.
2. The accuracy of the values should be at least 8 significant digits.
3. The matrix elements that it reads are: P_{11}, P_{12}, P_{22}, P_{33}, P_{34}, P_{44}. If the input matrix has other elements, matrix-reading part of the code must be modified.

Errors

Possible errors that the code may produce are:

- 'Trouble in GRAYOPT: ray/particle number mismatch.' – Number of particles exceeds the number of rays.
- 'Trouble in GRAYOPT: internal waves notably inhomogeneous.' – Maximum chord number should be zero if the imaginary part of the refractive index of the particle > 0.05.
- 'Trouble in GRAYOPT: random sphere type out of range.' – Sphere type not 1 (for general mode) or 2 (for concave-hull mode).
- 'Trouble in GRAYOPT: standard deviation .le. 0.' – Relative standard deviation of the radius is non-feasible.
- 'Trouble in GRAYOPT: inconsistency of H-G asymmetries.' – Problems with the D-H-G parameters (g1 < g2, g1 > 1, g2 < -1, g > g1, or g < g2, where g = asymmetry parameter, g1 = forward asymmetry, and g2 = backward asymmetry)
- 'Trouble in GRAYOPT: correlation function unknown.' – Correlation function value outside the options.
- 'Trouble in GRAYOPT: cflg .eq. 1 and minimum degree .lt. 2. – The correlation function value = 1 and minimum degree in C_1, C_2, C_3 < 2.
- 'Trouble in GRAYOPT: input angle .le. 0. .or. .gt. 180' – The correlation function value < 2 or the correlation angle outside the range 0-180 degrees.
- 'Warning in GRAYOPT: correlation angle will differ from input value. Set minimum degree to 0 and 'maximum degree .gt. (300 deg)/(input value).' – minimum degree in C_1, C_2, C_3 > 0 or maximum degree in C_1, C_2, C_3 < 300/Corr, Corr = Correlation angle for C_2 autocorrelation.

- 'Trouble in GRAYOPT: maximum degree .gt. 256.' - Maximum degree in C_1, C_2, C_3 > 256.
- 'Trouble in GRAYOPT: minimum degree .lt. 0.' - Minimum degree in C_1, C_2, C_3 < 0.
- 'Trouble in GRAYOPT: minimum degree .lt. maximum degree.'- Minimum degree in C_1, C_2, C_3 < Maximum degree in C_1, C_2, C_3.
- 'Trouble in GRAYOPT: number of triangle rows .gt.180.' - Number of triangle rows in an octant exceeds 180.
- 'Trouble in GRAYOPT: negative Legendre coefficient.' – Another problem with the degrees in C_1, C_2, C_3.

Output data

The output data consists of four files:
1. The input data
2. Scattering parameters etc.
3. Phase function and polarization degree
4. The full scattering matrix

The list of the contents of the output file **#1**:

rflg	=	Geometric optics (1), diffraction (2), or ray optics (3)
dflg	=	Diffraction: G-spheres (1) or equiv. spheres (2)
gflg	=	General (1) or concave-hull mode (2)
cflg	=	Correlation function (1=power law, 2=Gaussian, 3=file)
rtflg	=	Diffuse scattering medium (1)
ieflg	=	Internal (1) or external diffuse scattering medium (2)
pflg	=	Scattering matrix: input (1), Rayleigh (2), D-H-G (3)
wavelen	=	Wavelength (in length units)
radius	=	Mean radius of the particle (in length units)
mmed	=	Refractive index of the medium
mre	=	Refractive index of the particle: real part
mim	=	Refractive index of the particle: imaginary part
mre/mmed	=	Relative refractive index of the particle: real part
mim/mmed	=	Relative refractive index of the particle: imaginary part
xa	=	Size parameter of the particle *(2*pi*radius/wavelen)*
xsigr	=	Relative std of size parameter of the particle *(xa*sig)*
abscf	=	Absorption parameter of the particle *(2*xa*mim)*
sig	=	Relative std of radius of the particle
beta	=	Gaussian random sphere parameter *(sqrt(log(sig^2+1)))*
rho	=	0?
nuc	=	Power law index for C_1 correlation
gami	=	Correlation angle for C_2 autocorrelation
elli	=	*2*sin(0.5*gami)*
lmin	=	Minimum degree in C_1, C_2, C_3
lmax	=	Maximum degree in C_1, C_2, C_3
omt	=	Diffuse-medium single-scattering albedo

whg	=	Weighted H-G parameter *((ghg-ghg2)/(ghg1-ghg2))*
ghg	=	Diffuse-medium asymmetry parameter
ghg1	=	Diffuse-medium forward asymmetry
ghg2	=	Diffuse-medium backward asymmetry
pmx	=	Diffuse-medium single-scattering maximum polarization
lenrt	=	Internal diffuse-medium mean free path (in length units)
xlenrt	=	*xa*lenrt*
taurt	=	External plane-parallel-medium optical thickness
ntr	=	Number of triangle rows in an octant
ntri	=	Number of triangles in the shape mesh *(8*ntr^2)*
nnod	=	Number of nodes in the shape mesh *(4*ntr^2+2)*

The list of the contents of the output file **#2**:
Geometric optics:

piomax	=	Maximum chord number in ray tracing
nray	=	Number of rays
npar	=	Number of sample particles
nray/npar	=	Number of rays per sample particles
ntheg	=	Number of scattering angle bins
xsize	=	Size parameter of a sphere with an equal projected area
ar	=	True projected area (in length units squared)
rhit	=	?
rmiss	=	?
hit	=	Percent of rays that hit the target
miss	=	Percent of rays that missed the target

Preliminary efficiencies
qextG	=	Extinction efficiency
qscaG	=	Scattering efficiency
qabsG	=	Absorption efficiency
qbackG	=	Backscattering efficiency

Waste efficiencies:
qinG	=	?
qoutG	=	?
qtriG	=	?
qtotwasteG	=	?
qtotG	=	Total efficiency

Renormalized efficiencies:
qextG	=	Sum of renormalized qscaG and qabsG
qscaG	=	Preliminary qscaG / preliminary qextG
qabsG	=	Preliminary qabsG / preliminary qextG
qbackG	=	Preliminary qbackG / preliminary qextG

Cross sections:
sextG	=	Renormalized qextG * ar

sscaG   = Renormalized qscaG * ar
sabsG   = Renormalized qabsG * ar
sbackG   = Renormalized qbackG * ar

gG   = Asymmetry parameter
mu_C   = Circular-polarization ratio for backscattering

The content of the output file **#3** and **#4** (the scattering matrices):

#3: θ, P_{11}, $-P_{12}/P_{11}$, P_{22}/P_{11}, P_{33}/P_{11}, P_{34}/P_{11}, P_{44}/P_{11}

#4: θ, P_{11}, P_{12}, P_{13}, P_{14}, P_{21}, P_{22}, P_{23}, P_{24}, P_{31}, P_{32}, P_{33}, P_{34} P_{41}, P_{42}, P_{43}, P_{44}