Reference Manual for SPECTRA ver. 10.0

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Contents

1. Introduction

This document describes the instruction to use the free software *SPECTRA*, a synchrotron radiation (SR) calculation code developed at SPring-8, and is located in "[SPECTRA Home]/help", where [SPECTRA Home] is the directory where *SPECTRA* has been installed.

All the pictures of the GUI windows in this document are those of the Microsoft Windows (Windows 7) version, but other versions (Mac OS X and Linux) have similar appearances.

In this chapter, brief explanations on the software and numerical implementation of SR calculation are given with a simple instruction of how to get started.

1.1. Overview

SPECTRA is an application software to calculate optical characteristics of radiation emitted from various synchrotron radiation (SR) sources such as bending magnets (BMs) and insertion devices (IDs, i.e., wigglers and undulators). In addition, IDs with arbitrary magnetic fields are available by importing the magnetic field data prepared by users. This makes it possible to estimate the real performance of the SR source by using the magnetic field distribution actually measured by a field measurement instrument such as a Hall probe.

In order to calculate the optical characteristics to estimate the performances of SR sources, a lot of parameters are required to specify the accelerator performances, SR source configurations, and observation conditions.

SPECTRA is equipped with a fully graphical user interface (GUI) which helps the user to specify these parameters. In addition, a simple plotter is included to verify the results of calculation graphically. These graphical parts are written in C++ with the wxWidgets GUI tool kit library [2]. For visualization of results of several kinds of calculation, the OpenGL graphic library [3] is used. Thanks to portability of wxWidgets and OpenGL libraries, *SPECTRA* will run on most of the popular platforms such as Microsoft Windows, Macintosh OS X (OS 9.x or earlier is not supported), Linux, and most unix-like operating systems. *SPECTRA* does not require any other commercial softwares or libraries.

The numerical part of *SPECTRA* is also written in C++ with the standard template library (STL). For wigglers and BMs, numerical implementation is based on the well-known expressions on SR [4]. As for SR emitted from an ideal undulator, the so-called far-field approximation can be used for fast computation. For more accurate evaluation, expressions on SR in the near-field region are used for numerical computation. In this case, characteristics of SR emitted from both the ideal- and arbitrary-field devices

can be calculated. For details of numerical implementation, refer to [1], [5].

Before ver. 7.2, the magnetic field was assumed to be constant in the transverse (*x*-*y*) plane. In other words, only the dipole components were taken into account. This considerably simplifies the numerical algorithm not only in the trajectory calculation but also in the spatial integration to take into account the electron beam emittance.

In ver. 8.0, an arbitrary magnetic field has been supported to enable the evaluation of the effects due to quadrupole magnets between undulator segments and the undulator natural focusing, which would be significant for low-energy electrons.

In ver. 9.0, an arbitrary electron bunch profile (transverse and longitudinal) has been supported. The user can import the bunch profile data of the electron beam either in the projected profile or in the marcroparticle coordinates in the 6-dimenional phase space, which is usually created by the start-to-end simulation for X-ray FELs.

In ver. 10.0, a new function to compute the photon flux density in the four dimensional phase space *(x, x', y, y')* has been implemented, which enables the rigorous estimation of the brilliance of typical SR sources and distribution of the photons at the source point to be utilized in other computer codes for ray-tracing simulation.

1.2. Type of SR Sources

Two kinds of SR sources are available in *SPECTRA*. One is a built-in SR source with an ideal magnetic field profile (sinusoidal for undulators/wigglers and uniform for bending magnets). The other is a custom SR source with an arbitrary magnetic field distribution specified by the user. Refer to Selection of the SR Source Type (5.6) for details.

1.2.1. Built-in SR Source

A number of SR sources are available in *SPECTRA* without any special configurations: conventional undulators, helical undulators, wigglers, bending magnets, etc. Calculations based on the Far Field Approximation (1.3.1) are available for the built-in SR sources.

1.2.2. Custom SR Source

Beside the built-in SR sources described above, it is possible to specify an arbitrary magnetic field distribution and create a customized SR source. Note that the Far Field Approximation (1.3.1) cannot be applied. Thus, a longer computation time will usually be needed for this type of SR source.

1.3. Numerical Methods for Characterization of SR

In order to perform an effective numerical computation, formulas to express the SR characteristics should be simplified as much as possible. There exist two numerical methods to formulate the analytical expressions on SR, i.e., "near-field" and "far-field" expressions. In both methods, the electron is assumed to be relativistic. Let $\boldsymbol{R}$ and $\boldsymbol{r}$ be the vectors directing from the origin of the SR source to the observer, and to the electron moving in the magnetic field of the SR source, respectively. In addition to the above two methods, a new function has been implemented in ver. 10, which makes it possible to characterize the SR at the source point.

1.3.1. Far Field Approximation

In the "far-field" expression, optical characteristics of radiation from SR sources are calculated with an assumption that $|\boldsymbol{R}|$ is much larger than $|\boldsymbol{r}|$. This also implies that the observation angle, i.e., an angle formed by the two vectors $\boldsymbol{R}$ and $\boldsymbol{r}$, is kept constant. This significantly simplifies the expressions on SR and thus enables a fast computation. For most purposes, such as evaluation of the photon flux passing through a slit and heat load on optical elements, this method is recommended and in fact enough.

1.3.2. Near Field Expression

No approximation is made in this method besides an assumption that the electron is relativistic. In other words, the observation angle is a function of the electron position, i.e., it varies while the electron travels in the SR source. If the distance between the SR source and observer is comparable to the length of the SR source itself, the near-field effect would not be negligible. Especially, the off-axis spectrum will be considerably different from that observed at the point infinitely far from the SR source.

1.3.3. Photon Distribution at Source Point

In the above two formulations, the angular (Far Field) or spatial (Near Field) profile of radiation is computed at a certain observation point located behind the SR source. In some cases, one needs to compute the photon distribution exactly at the source point, which is usually the center of the SR source. This means that the distance from the source to the observer is zero, i.e., $|\boldsymbol{R}| = 0$. Computing the SR properties under such a condition is not possible in a straightforward way, but requires another numerical operation to propagate the radiation from the observation point back to the source point. *SPECTRA* is equipped with a number of numerical methods to enable this function.

1.4. Getting Started

In order to quickly get started with *SPECTRA* for SR calculation, follow the steps below.

(1) Open a parameter file by running [File]-[Open Parameter File] command. You can also run [File]-[Create New] command to start with a new parameter set.
(2) Select a type of SR source from submenus in [Configurations]-[Light Source]-[Source Type].
(3) Select a type of calculation from submenus in [Select Calculation]. The type of calculation is classified according to the “main output item” (flux, power density, etc.) and “dependence” (energy, spatial, etc.).
(4) Edit the parameters in the GUI windows if necessary.
(5) Run [Run]-[Start Calculation] command to start a calculation with current parameters shown in the GUI windows. Then a file-selection dialog box pops up. Enter a file name to save the calculation results. The output data are saved in a file with some suffix depending on the type of calculation.
(6) In order to perform more than one calculation, run [Run]-[Create Process] command to create a “process”, which saves all the parameters in the configuration GUI windows to temporary memory and adds the created process to the current calculation list.
(7) Repeat it until all the desired calculation processes are created. Then run [Run]-[Start Calculation] command to start the calculations in series. You can also create a calculation process by scanning a parameter. Refer to Scanning a Parameter (2.4) for details.
(8) A GUI window with a progress bar pops up to inform the user of the calculation status.
(9) In order to verify the calculation results after completion of the calculation, run [Open Utility]-[Simple Plotter] command, select the name of the output file and item(s) to check, and click [Plot] button to create a graphical plot. Refer to Visualization of Calculation Results (2.2) for details.

2. Instructions for Use

This chapter describes general instructions for use of *SPECTRA*. In addition to the method to start a simple calculation, convenient functions such as parameter scanning and importing/exporting the calculation configurations are presented.

2.1. Simple SR Calculation

Before starting any calculation in *SPECTRA*, one needs to open a parameter file, edit the parameters and select the calculation type.

2.1.1. Open a Parameter File

Upon being started, *SPECTRA* tries to load parameters from the parameter file that was opened last time. If successful, the parameters are shown in the GUI windows. If *SPECTRA* is run for the first time after installation, nothing will be shown. Open a *SPECTRA* parameter file by running [File]-[Open Parameter File] command. In the initial setting, the parameter files are found in the directory "[SPECTRA Home]/prm" with a default suffix "prm", where "[SPECTRA Home]" is the directory where *SPECTRA* has been installed.

2.1.2. Select Calculation Type

The type of calculation can be selected by running one of the submenus in [Select Calculation] on the main menu bar as shown in Figure 2.1. For details of each calculation type, refer to Calculation Type and Output Items (chapter 3).

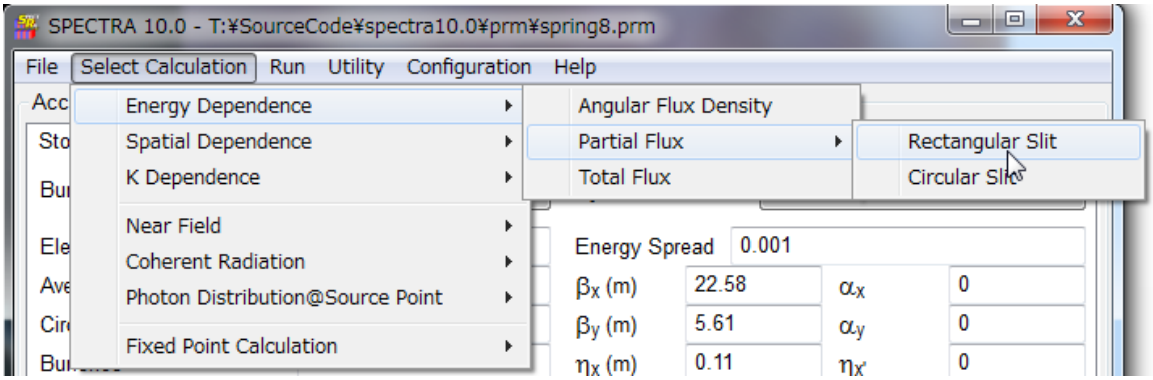


Figure 2.1 Selection of the calculation type.

2.1.3. Edit Parameters

Parameters necessary for SR calculation are edited in the configuration GUI windows. In general, there are several ways to specify a certain set of parameters. For example, the horizontal and vertical emittance values can be calculated once the natural emittance and coupling constant are specified, and vice versa.

It is in principle possible to select either of the two parameter sets in order to express the electron-beam quality.

In *SPECTRA*, the natural emittance and coupling constant are specified by the user (input parameter), and the horizontal and vertical emittance values are calculated internally (output parameter). All the input parameters are shown in the text entry boxes in the GUI windows and can be edited. Once they are edited, the related output parameters are calculated automatically and the values are updated. Also refer to Figure 2.2.

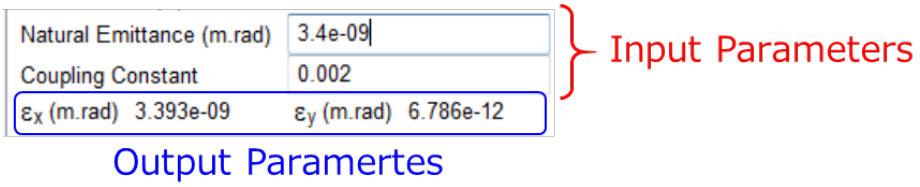


Figure 2.2 Input and output parameters shown in the GUI window.

2.1.4. Starting a Calculation

After completion of specifying the input parameters, run [Run]-[Start Calculation] command to start a single calculation. Input a data name in the file-selection dialog box that pops up. A GUI window pops up to indicate the calculation status as shown in Figure 2.3. In order to cancel the calculation, click [CANCEL] button.

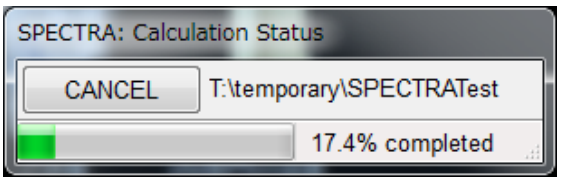


Figure 2.3 Progressbar to indicate the calculation status.

Notes for LINUM users: The progress bar and message to indicate the calculation status do not appear in the LINUX version because of the GUI library problem, which has not yet been solved. Instead, the status is indicated in the terminal (console) window where *SPECTRA* has been launched.

2.2. Successive Calculations

In order to to specify a number of calculations with different sets of parameters, run [Run]-[Create Process] command every time you finish specifying all the parameters. Then input a data name in the file-selection dialog box that pops up. A GUI window pops up as shown in Figure 2.4 to show the calculation list currently saved in a temporary memory. Repeat it until all the calculations are specified. Click [Remove] button to delete the selected calculation, or [Clear] to clear out all the calculations.

Next run [Run]-[Start Calculation] command. The calculations in the list are performed in series. The calculation status is indicated in the progressbar in the GUI window. Click [CANCEL] button to cancel the calculation currently in progress, or [CANCEL ALL] button to cancel all the remaining calculations.

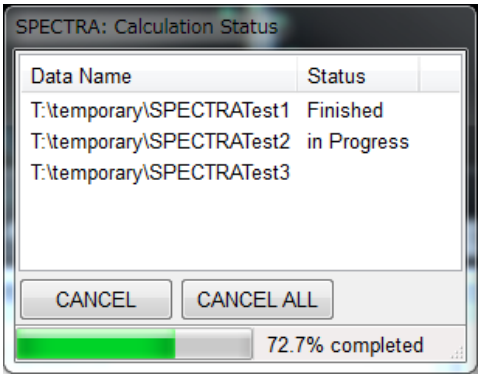


Figure 2.4 Progressbar to indicate the calculation list and status.

2.3. Scanning a Parameter

Besides the Successive Calculations (2.2) scheme described in the previous section, it is possible to specify a lot of calculation processes at once by scanning a certain parameter.

2.3.1. General Instruction

In order to scan a parameter, select the text entry box showing the parameter to be scanned in the GUI panels and right-click (double-click in MacOSX) it. Run [Scan This Parameter] command in the popup menu as shown in Figure 2.5. Then a dialog pops up to specify the parameters for scanning as shown in Figure 2.6.

Enter the initial and final values and number of points for scanning. For several parameters that are to be specified by an integer, scanning interval should be specified instead of the number of points. If “Logarithmic Step” option is checked, the parameter is to be varied so that its logarithm changes in a regular step. To be more specific, the ratio between two successive parameter values is kept constant.

If the target parameter refers to one of the X (horizontal) and Y (vertical) components, such as β_y (vertical betatron function) or x (horizontal observation position), it is possible to scan two parameters in the both directions. To be more specific, if [Scan X&Y Parameter] command is available, 2-D (X and Y) scan is possible. In such a case, specify the scanning parameters in the both directions in the configuration window.

In order to create the scanning calculation process, click [OK] button. Input a data name in the file-selection dialog box that pops up. Then the specified parameters are saved in a temporary memory and

the scanning process is saved in the calculation list (Figure 2.4). Run [Run]-[Start Calculation] command to start the calculation. The method of how to save the scanning result depends on the type of calculation (chapter 4). Namely, it depends on whether the selected calculation type belongs to Fixed Point Calculation or not (general calculations). Refer to the following sections for details.

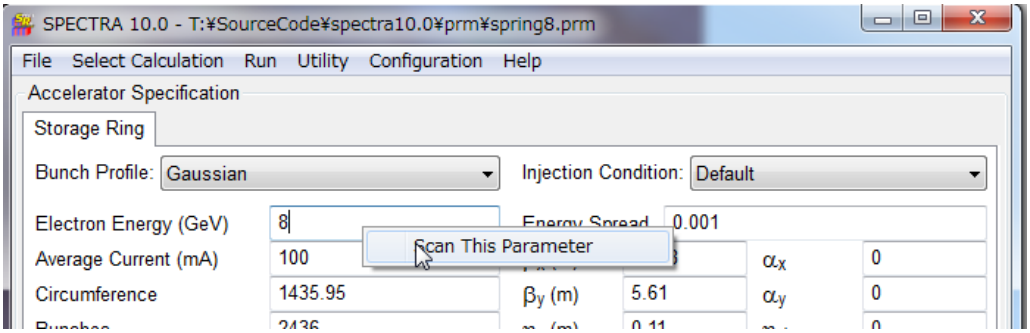


Figure 2.5 Scanning a parameter. In the above case, "Electron Energy" is to be scanned.

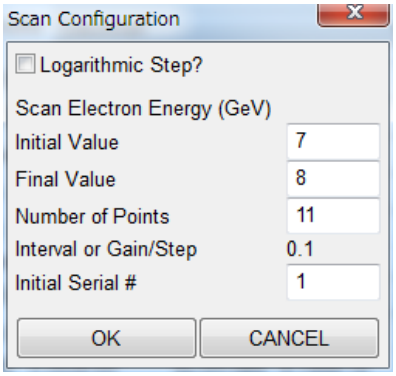


Figure 2.6 Configuration window to create a scanning process.

2.3.2. General Calculations

The calculation results are saved as follows. First, a directory with the data name specified in the file-selection dialog box is created. Each output file is saved in this directory with a serial number being attached. For example, if "[Data Directory]/test" is selected as the data name and "Scanning Points" and "Initial Serial #" parameters are set to 10 and 1, respectively, then output files with the names from "[Data Directory]/test/test-1[.suffix]" to "[Data Directory]/test /test-10[.suffix]" are created, where [.suffix] is the suffix defined by the selected type of calculation.

Besides the above output files, a header file containing the scanning condition is created in the parent directory of the data directory where the output files are saved. In the above example, a file with the name "[Data Directory]/test.hdr" is created. This file can be used to create an animation file from the output files as described in Visualization of Scan Calculation (section 3.3).

2.3.3. Fixed Point Calculation

If the current calculation type belongs to Fixed Point Calculation, the calculation results are saved in a single file with the name specified by the user, which has a spreadsheet file format, with the 1st (and 2nd in 2-D scan) column denoting the parameter(s) being scanned. Other columns denote the output items that depend on the selected type of calculation. Note that the header file described above is not created in this case.

2.4. Exporting and Importing the Configurations

All the parameters and configurations for the calculation can be exported to an external file, which can then be utilized later in *SPECTRA*. Run [Run]-[Export Calculation Settings] command to export the current parameters, and then input a file name in the file selection dialog box. Even if more than one calculation is specified by the procedure explained in sections 2.2 and 2.3, all the configurations are saved in a single file. The exported file (configuration file) is a simple text file with an ASCII format, and thus can be easily checked and edited if necessary. For details of the configuration file, refer to ***. In order to import the configuration file, run [Run]-[Import Calculation Settings]. Then the GUI window as in Figure 2.4 pops up to show the imported calculation list.

2.5. Parameter Set

The “Parameter Set” is a group of input parameters, configurations and options bundled together. There are four types of parameter sets in *SPECTRA*.

2.5.1. Accelerator Parameter Set

The parameter set to specify the accelerator performance. Detailed descriptions on individual parameters are given in Accelerator Specification (Chapter 4).

2.5.2. Light Source Parameter Set

The parameter set to describe the SR source. Detailed descriptions on individual parameters are given in Light Source Description (Chapter 5).

2.5.3. Calculation Control Parameter Set

The parameter set to configure the calculation conditions. Detailed descriptions on individual parameters are given in Calculation Configurations (Chapter 6).

2.5.4. Beamline Parameter Set

The parameter set to bundle the above 3 parameter sets to specify the “beamline” in a SR facility.

2.5.5. Operation of the Parameter Set

The parameter sets loaded from the *SPECTRA* parameter file are listed in the submenus in [Configuration] menu. By selecting one of the submenus, related parameter set is selected and the parameters in the GUI windows are updated with the parameters in the selected parameter set. The submenus of [Configuration] menu have three commands related to operation of the parameter set as explained below.

Duplicate

A new parameter set is created by running [Duplicate] command as a copy of the current parameter set.

Change Name

The name of the current parameter set is changed by running [Change Name] command. Input a new name in the text entry dialog box.

Delete

The current parameter set can be deleted by running [Delete] command. At least one parameter set should be left.

Sort

The parameter sets are sorted by running [Sort (A to Z)] or [Sort (Z to A)] command accordingly.

3. Visualization of the Computation Results

SPECTRA is equipped with several functions to visualize the computation results. Details of these functions are explained in this chapter.

3.1. Visualization of Calculation Results

After completion of a calculation, the output data can be plotted graphically to verify the results. Configurations to plot the calculation results are available in the GUI window as shown in Figure 3.1, which pops up by running [Open Utility]-[Simple Plotter] command.

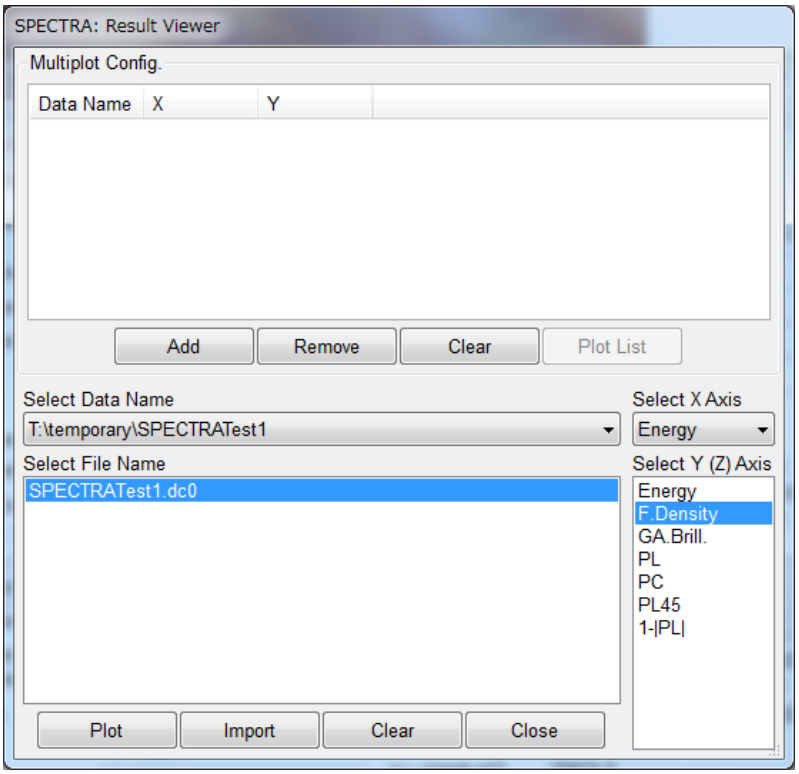


Figure 3.1 GUI window for configuration of plotting the calculation results.

3.1.1. Single Data Set

In order to plot the calculation results, specify the data name, file name and item(s) for X/Y axis in the GUI window. Refer to the followings for details.

Select Data Name

The data names, specified in the file-selection dialog box just before starting a calculation, are stored in this list. Select a desired one for plotting. The data name is automatically added to the list after completion of a calculation. It is also possible to add a data file manually. To do so, click [Import] button and select the file name in the file-selection dialog box that pops up.

Select File Name

In several types of calculation, a certain number of files are created to save the calculation results. For example, the spatial dependence along the x- and y- axes are saved in two files separately, i.e., "****.dtx" and "****.dty", respectively, where "****" means a data name. Select desired file(s) for plotting.

Select X/Y or Z Axis

In order to specify the abscissa (X Axis) and ordinate (Y Axis) of the plot, select a desired item in these lists. Multiple selections are allowed for Y Axis, which results in a multiple plot. If the calculation result is in a 3-dimensional (3-D) form (e.g., [Spatial Dependence]-[Cartesian Mesh] is selected), the X and Y axes are automatically chosen, so select only the item for the Z axis.

After specification of all the items above, click [Plot] button to create a graphical plot as shown in Figure 2.6. To clear all the data names in list, click [Clear] button.

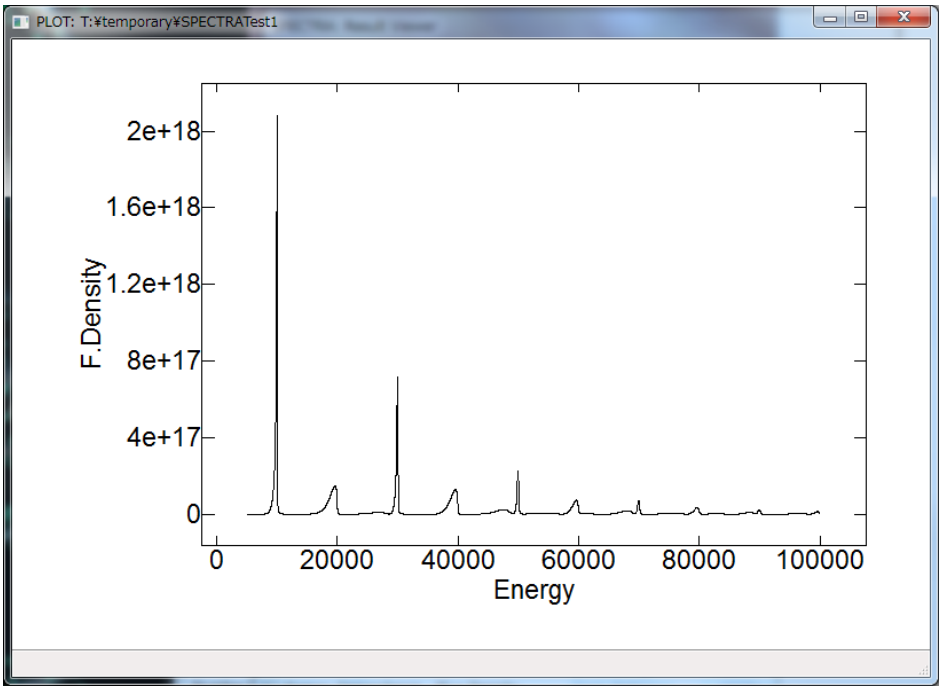


Figure 3.2 Example of a graphical plot to view the calculation result.

3.1.2. Multiple Data Sets

Besides creating the plot with the single data set explained above, more than one data set can be plotted in a single window. To do so, click [Add] button after specifying all the items necessary to create a plot with a single data set. The contents of the plot are listed in the top box. After adding all the data sets, click [Plot List] button to create the plot with multiple data sets. Click [Remove] button to delete the selected plot, and [Clear] button to clear out the plot list.

3.2. Editing the 2-D Plot

In the 2-D graphical plot as shown in Figure 2.6, a number of commands are available to modify the appearance of the plot. In order to edit the plot, drag, left-click, or right-click the plot window and run one of the commands, which are explained in the following sections.

3.2.1. Zoom

In order to expand or shrink the plot, drag the range of interest. Then in the pop-up menu, run [Zoom In] to expand, and [Zoom Out] to shrink.

3.2.2. Specify and Read a Point

In order to get the coordinate of a certain point in the plot, left-click the pixel near that point. Then, the X (abscissa) and Y (ordinate) coordinates are indicated in the format x=****, y=**** in the status bar located on the bottom of the plot.

3.2.3. Commands Available by Right-Click

A number of commands are available by right-clicking the plot, which are explained as follows.

Log/Linear Scale: X/Y Axis

The scale of the abscissa or ordinate can be changed from logarithmic to linear, or vice versa.

Initialize Scale

Changes the plotting range to the original one.

Edit Options

Open a dialog window to edit the details of the plot. Refer to Plot Options (section 3.2.4) for details.

Line/Symbol/Line+Symbol

Selects the method of how to indicate and connect the points in the plot.

Print Preview/Printer Setup

Preview the plot or setup the printer for printing the plot.

Close

Close the plot window.

3.2.4. Plot Options

The details of the plot, such as the color, symbol type, plotting range, offset, and status can be specified in the dialog box shown in Figure 2.7, which pops up by running [Edit Options] command in the pops when right-clicking the plot.

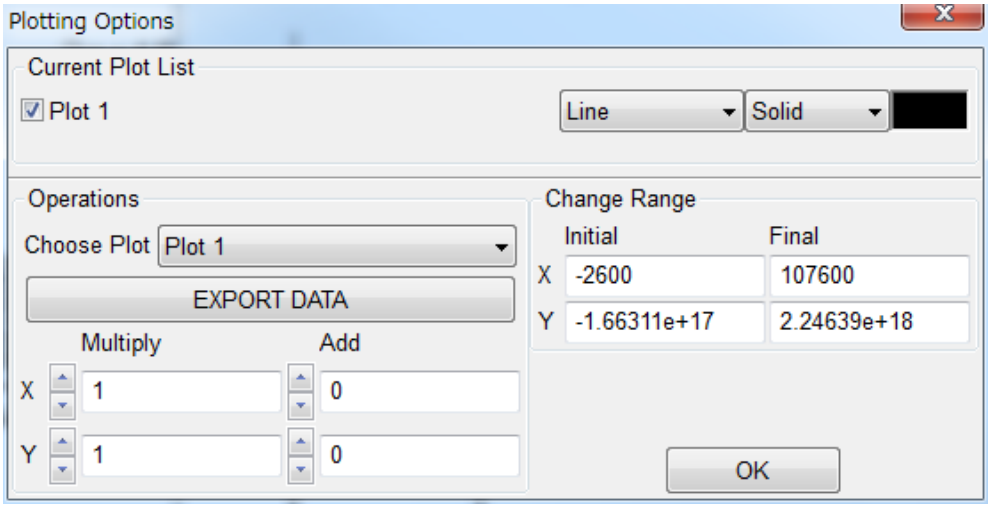


Figure 3.3 GUI window to edit the details of the plot.

Current Plot List

Configures the appearance of the plot. The checkbox in the left side specifies if the plot is shown or hidden. In the two choice boxes in the right side, the plot type and symbol can be selected. The plot color can be chosen by left-clicking the painted box at the right side.

Operations

In order to improve the appearance of the plot, especially to compare more than one plot, arithmetic operations are possible. To do so, choose the plot in the top choice box, and input the offset to be added and coefficient to be multiplied.

EXPORT DATA

Exports the numerical data currently chosen in the [Choose Plot] list box. Input a file name to save the data in the file-selection dialog box that pops up.

Change Range

Specifies the plotting range in X and Y axes.

3.3. Editing the 3-D Plot

In the 3-D plot, selection of the plot type (Surface, Contour, or Contour+Surface) is the only operation available, unlike the 2-D plot. Choose the desired plot type in the pop up menu, which is available by right-clicking the plot.

3.4. Visualization of Scan Calculation

In the parameter scanning explained in section 2.3, all the output files have the identical format in terms of the output items and dependency. Thus it is possible to create an "animation" by creating a graphical plot for each output file as a slide of the animation. In order to create an animation from the scanning calculation results, run [Open Utility]-[Visualization of Scan Results] command to open a GUI window as shown in Figure 2.9. Then, follow the instructions below.

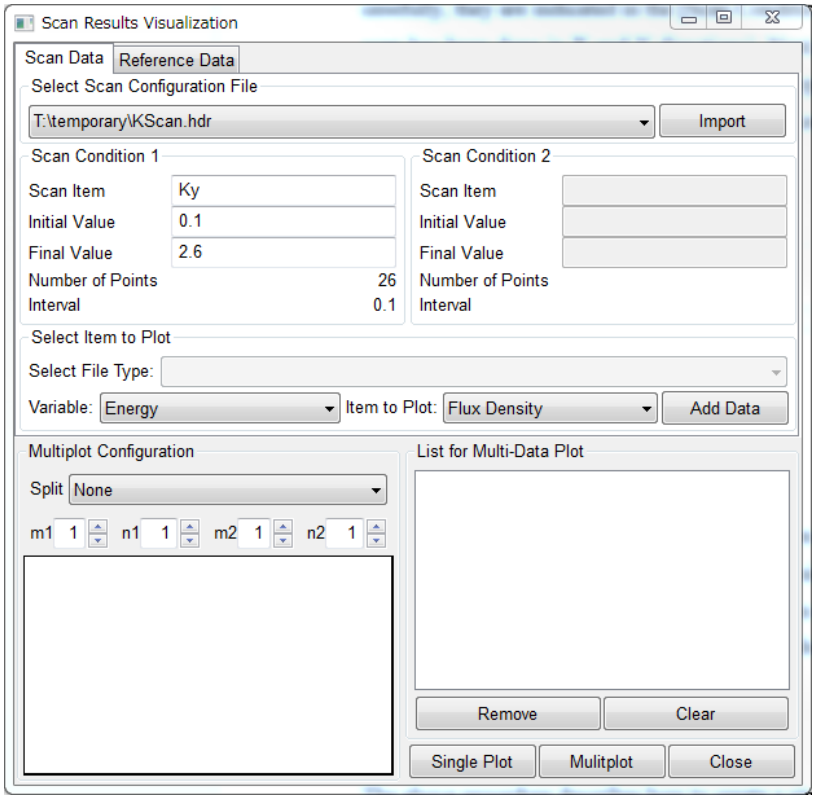


Figure 3.4 Configuration window to create an animation from scanning results.

3.4.1. Single Plot with a Single Data Set

First, import the header file ("***.hdr", refer to section 2.3) that contains the scanning conditions by clicking [Import] button in the [Select Scan Configuration File] group box in the [Scan Data] tab window, and specify its location in the file-selection dialog box. If all the scanning conditions are loaded successfully, they are indicated in the [Scan Condition 1] group box (and also in [Scan Condition 2], if the scan has been done in X and Y directions). Next, select the item to be plotted in [Select Item to Plot] group box. In some cases, selection of the file type ([Select File Type]) is required. Then click [Single Plot] button to create a GUI window that visualizes the output files as an animation (animation GUI

window). Figure 3.5 shows an example of the animation GUI window. It is possible to configure the animation with a number of commands available in the GUI window. For details, refer to section 3.5.

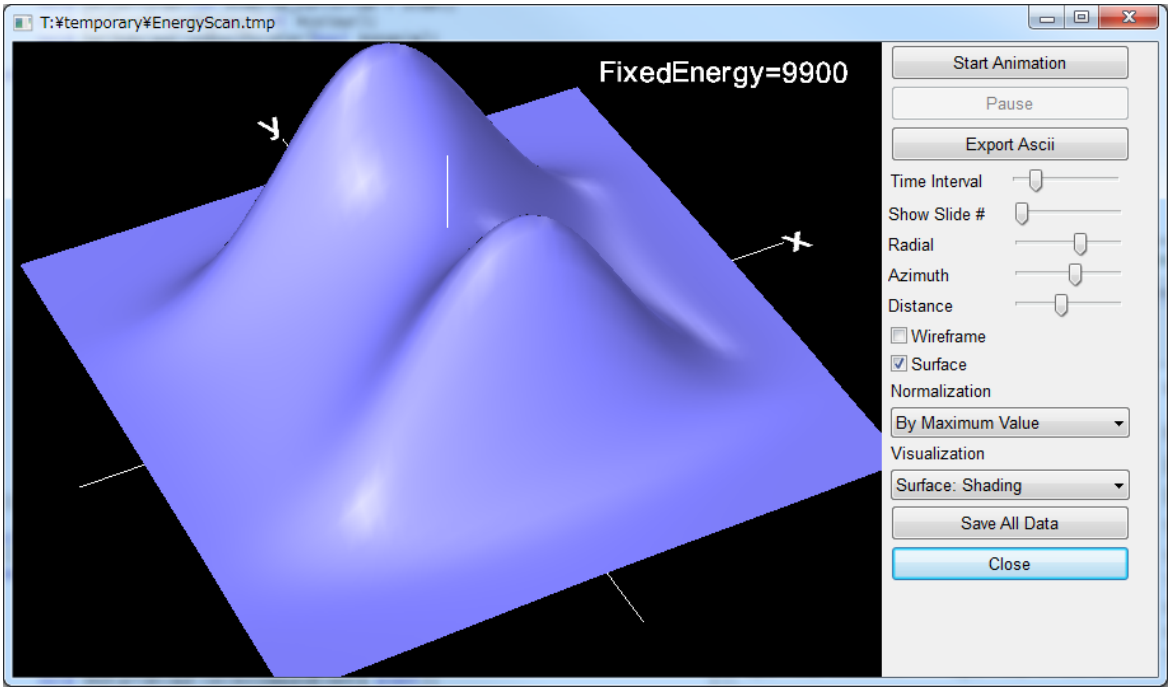


Figure 3.5 An animation GUI window to visualize the scanning results.

Besides the scanning results, a simple calculation result (referred to as [Reference Data]), which is obtained by a single calculation but not by the scanning option, can be also plotted. To do so, click [Import] button in the [Select Reference File] group box in the [Reference Data] tab window, and specify the file location. In the same manner as that described above (using the header file), you can set up the plot by selecting the item to be plotted.

3.4.2. Single Plot with Multi Data Set

The above procedure describes how to create a single plot, namely, a plot containing a single data set. In order to create a plot showing more than one data set (multi data set), click [Add Data] button in the [Select Item to Plot] group box in either of the two tab windows ([Scan Data] or [Reference Data]), then the data name is stored in the list box in [List for Multi-Data Plot] group box. After specifying all the data sets to plot, click the [Single Plot] button to create the animation GUI window. Note that even after creating the plot, the data set list remains in the list box. In order to create a single plot with a single data set afterwards, click [Clear] button to clear the list.

3.4.3. Multiplot

The plot with multi data set explained in the previous section is convenient to compare the behavior of different items having identical formats and similar data ranges (scale of X and Y axes). On the other hand, one may need to compare the behaviors of different items having different formats and/or data ranges. In such a case, it is not a good idea to plot all the data sets in the same plot. Instead, *SPECTRA* offers a function to create a GUI window composed of a number of plots (multiplot window) having different formats and data ranges. The configurations to create the multiplot window are summarized in the [Multiplot Configuration] group box, and the instructions are given in the following sections.

How to Partition the Window

In order to specify the number of plots, the client area should be partitioned, which is actually done according to [Split] option and [Matrix Size] parameter. The [Split] option determines how to divide the client area into two divisions that can be resized, while the [Matrix Size] parameters determine the number of columns and rows in each division.

In Figure 2.10, “Horizontally” is selected as [Split] option and [Matrix Size] parameters are set as m1=1, n1=2, m2=2, and n2=3, respectively. In this case, the client area is split into two divisions by the horizontal sash, which can be dragged to resize the divisions. The divisions are further divided into subdivisions, according to the matrix size (m1, n1 for subdivision 1 and m2, n2 for subdivision 2). The subdivisions cannot be resized and regularly arranged inside the division. The plot is created inside each subdivision, so 8 plots will be created in this case.

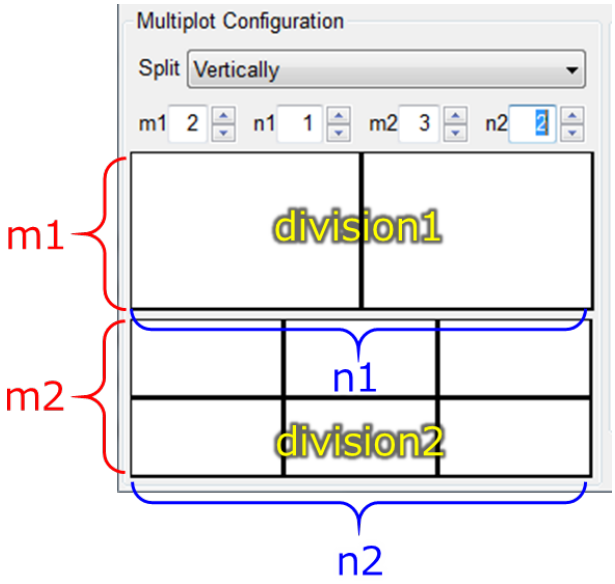


Figure 3.6 Configuration of the multiplot using [Split] option and [Matrix Size] parameter.

Data Allocation and Data Dump

After partitioning the client area, respective data set should be allocated to each subdivision. In order to do so, right-click the area of desired subdivision, then a popup menu appears. Select [Allocate current parameter set here] menu to allocate the animation data to the selected subdivision with the parameters (Data File, Sub Category, and Items for X,Y,Z Axes) currently selected. If successful, the area of the selected subdivision is painted gray. If [Clear] is selected from the popup menu, all the data allocations are released. After allocating the animation data to all the subdivisions, click [Multi] button to start to dump the data and create the plot window.

3.5. Commands in the Animation GUI Window

The animation GUI window, as shown in Figure 3.5, accepts a number of commands to control the animation, which can be classified into two groups: individual and common groups. The former refers to the individual commands that apply only to a certain plot (target plot) and can be run by right-clicking the area of the target plot. The latter refers to the common commands that apply to all the plots and the GUI controls to run the common commands are placed at the right side of the window.

3.5.1. Individual Commands

Table 3.1 summarizes the individual commands, which is available by right-clicking the client area of the target plot.

Table 3.1 Functions of GUI controls in the animation GUI window. *Not available in the 3-D plot.

Menu	Function
Log/Linear Scale: X/Y Axis*	Changes the X/Y axis scale from linear to logarithmic or vice versa.
Set X/Y Range*	Changes the plotting range in the X/Y axis. Input minimum and maximum values in the dialog box.
Initialize X/Y Range*	Changes the plotting range in the X/Y axis to the original values.
Export ASCII	Exports the plot data to a text file with an ASCII format. If the plot contains more than one data set, all of them are saved in the file with a line indicating the start and end of individual data set.
Change Color	Changes the plot color. If the plot contains more than one data set, the colors of individual plots can be specified.

3.5.2. Common Commands

Table 3.2 summarizes the common commands, which can be run by the GUI controls bundled in the right side of the window.

Table 3.2 Functions of GUI controls in the animation GUI window. *Functionally in the 3-D plot.

GUI Control	Function
Start Animation	Starts the animation. Disabled while it the animation in progress.
Pause/Resume	Stops or resumes the animation. Enabled only while the animation is in progress.
Time Interval	Specifies the time interval between slides. Increasing this value makes the animation slower. The actual time interval is dependent on the computer environment such as the platform and CPU.
Show Slide #	Shows the graphical plot corresponding to the selected slide number.
Radial, Azimuth, Distance*	Changes the direction of the plot or the distance from the viewpoint to the plot origin.
Wireframe*	Shows a wireframe on the plot.
Surface*	Shows a surface plot.
Normalization	Selects the method to normalize the plot. [At Each Step] means that the item is normalized by the maximum value in the current plot (slide), while [By Maximum Value] means that the items is normalized by the maximum value among the whole data.
Visualization*	Specifies the appearance of the plot. [Surface: Color Map] or [Surface: Shading] shows the surface plot painted with a color map or illuminated by an external light source, while [2D: Color Map] or [2D: Monochrome] shows the color or monochrome contour plot.
Save All Data	Saves the current data and settings to a file. The animation can be reproduced later by running [File]-[Open SPECTRA Output]-[Visualization File] command.
Terminate	Terminates the animation. Enabled only while the animation is in progress.

4. Calculation Types and Output Items

There are a number of characteristics that specify the performance of SR, e.g., wavelength, source size and angular divergence, photon flux, radiation power, polarization, and so on. Although an infinite number of formats can be considered in order to output these characteristics as numerical data, *SPECTRA* offers several standard formats (calculation types) depending on the purpose of SR calculation. In this chapter, the details of calculation types are explained.

4.1. Classification of Calculation Type

Before starting any calculation in *SPECTRA*, the user is requested to run one of the submenus of [Select Calculation] menu command in order to select the calculation type, which is classified by a number of categories such as the numerical method, dependency, main output item, and other procedures. For example, by selecting [Near Field]-[Energy Dependence]-[Spatial Flux Density], the spatial flux density (main output item) and related items are calculated as a function of photon energy (dependency) based on the near-field expression (numerical method).

Table 4.1 summarizes the calculation types implemented in SPECTRA. Each calculation type can be selected by running one of the submenus of [Select Calculation] menu command, which are indicated by “Main Menu” in the table. Most of them have submenus as indicated in “Submenu 1~3”, which specify the calculation configurations in more detail. The method column in the table indicate the numerical method to be applied for individual calculation types.

Note that not all of the calculation types shown in Table 4.1 are always available, but the availability depends on the type of the SR source and what kinds of options are enabled. For example, “K Dependence” calculations are obviously not available for bending magnets. However, the user does not have to take care of the availability, because *SPECTRA* automatically disables the menu commands that are not available once the calculation conditions are changed.

The classifications of calculation types described above are explained in the following sections, together with the descriptions of categories for each classification. Note that parameters and configurations necessary to specify the calculation conditions are explained later in chapter 7, and are not described here. Also note that the calculations, which are based on the numerical method referred to as “Source Point” in Table 4.1, require special numerical operations, and may be less familiar to the users compared to other calculations. So an introduction and explanations are described in more detail separately in section 4.3.

Table 4.1 Calculation types implemented in SPECTRA, which are classified by the dependence, main output item, and numerical method. *Not available in "Coherent Radiation".

Main Menu	Submenu (1)	Submenu (2)	Submenu (3)	Method
Energy Dependence	Angular Flux Density			Far Field
	Partial Flux	Rectangular/Circular Slit		
	Total Flux			
	Characteristics			
Spatial Dependence	Angular Flux Density	Along Axis/Cartesian Mesh /Cylindrical Mesh		
	Angular Power Density			
	Resolved Power Density			
K Dependence	Simplified Calculation	Brilliance at Peak Energy		
		Characteristics		
		Brilliance Curve		
	Flux at Fixed Energy	Angular Flux Density		
		Partial Flux	Rectangular/Circular Slit	
	Flux at Peak Energy	Angular Flux Density		
		Partial Flux	Rectangular/Circular Slit	
	Power	Angular Power Density		
		Partial Power	Rectangular/Circular Slit	
Near Field/ Coherent Radiation	Energy Dependence	Spatial Flux Density		Near Field
		Partial Flux	Rectangular/Circular Slit	
	Spatial Dependence	Spatial Flux Density	Along Axis/Cartesian Mesh /Cylindrical Mesh	
		Spatial Power Density		
	Radiation Field by a Single Electron*	Time Dependence		
		Complex Amplitude Spatial Profile		
Photon Distribution at Source Point	Wigner Function	Energy Dependence		Source Point
		K Dependence		
		Brilliance Curve		
		Phase-Space Profile	X-X' Plane (Sliced)	
			X-X' Plane (Projected)	
			Y-Y' Plane (Sliced)	
			Y-Y' Plane (Projected)	
			(X,X',Y,Y') Space	
	Spatial Profile			
Fixed Point Calculation	Flux	Angular Flux Density		Far Field
		Partial Flux (Rectangular Slit)		
		Partial Flux (Circular Slit)		
		Total Flux		
	Power	Angular Power Density		
		Partial Power (Rectangular Slit)		
		Partial Power (Circular Slit)		
	Brilliance by Gaussian Approximation			
	Characteristics			
	Near Field/ Coherent Radiation	Spatial Flux Density		Near Field
		Partial Flux (Rectangular Slit)		
		Partial Flux (Circular Slit)		
		Spatial Power Density		
		Partial Power (Rectangular Slit)		
		Partial Power (Circular Slit)		
	Wigner Function	Sliced		Source Point
		Projected (X)		
		Projected (Y)		
		Decoupling Factor		
		Degree of Coherence		

4.2. General Classification

This section describes the general classification by the numerical method, dependence, and main output item. Other classification by other special categories are discussed later.

4.2.1. Classification by the Numerical Method

As mentioned in section 1.3, the numerical methods implemented in *SPECTRA* can be classified into three types: far field approximation, near field expression, and photon distribution at the source point. Among them, computations based on the far field approximation are the fastest and in most cases accurate enough. So, the user is strongly recommended to try this option first, if possible. Note that the term "Far Field" is not explicitly indicated in the menu command even for the calculations based on the far-field approximation. This is because the early version of *SPECTRA* was equipped only with the computation based on the far-field approximation, and the other numerical methods were not available. As for the photon distribution at the source point, refer to section 4.3.

4.2.2. Classification by the Dependence

In *SPECTRA*, the main and related output items (refer to the next section) are usually calculated as a function of certain variable, which is referred to as "Dependence". For example, "Energy Dependence" means that output items are calculated as a function of the photon energy. Note that the calculations under "Fixed Point Calculation" are different in the point that the calculation is done at a fixed calculation condition (photon energy, observation position etc.), and the output file is not created but the results are shown in Calculation Configurations GUI window (chapter 7), after the computation is completed.

4.2.3. Classification by the Main Output Item

The main output item specifies one of the physical quantities that characterize the light source performance of SR. Note that other properties that are relevant to the main output item are calculated simultaneously as "output items", without additional numerical cost. For example, "Angular Flux Density" as the main output item means that the degree of polarization is calculated as well. For meanings and units of the output items (main and related) used in *SPECTRA*, refer to section 9.1.

In most cases, the main output item is selected from the properties related to the photon flux or radiation power: angular/spatial flux density, partial/total flux, angular/spatial power density or partial power. Refer to section 4.5 for other main output items available in SPECTRA.

4.3. Calculations at the Source Point

In the case of calculations based on the far-field approximation or near-field expression, we assume that the observation point is located behind the SR source. In *SPECTRA*, characterization of radiation exactly at the source point is also possible in terms of two items: Wigner function and spatial profile.

4.3.1. Wigner Function

The photon flux density in the phase space spanned by the spatial $(x, y) = \boldsymbol{r}$ and angular $(x', y') = \boldsymbol{r}'$ coordinates, which is referred to as the phase-space density and denoted by $d(x, y, x', y')$, is an important physical quantity to characterize SR as a light source. Its maximum value, which is known as brilliance (also refer to section 9.1.6 for details) or brightness, gives the information of how many coherent photons are available. Its distribution in the phase space is necessary to carry out the ray-trace simulation based on the geometrical optics.

It is worth noting that the angular profile of SR in the far-field region is obtained by integrating $d(x, y, x', y')$ over (x, y), while the spatial profile in the near-field region is obtained by integrating over (x', y'). Also note that these spatial and angular profiles can be computed directly from analytical formulas based on classical electrodynamics. However, there is no analytical method to calculate $d(x, y, x', y')$ directly from the first principle. The Wigner function $W(x, y, x', y')$ is introduced in SR formulation to solve this problem and makes it possible to compute $d(x, y, x', y')$ from the complex amplitude of radiation.

SPECTRA is equipped with several functions to compute the phase-space density not only for the single electron, but also for more practical conditions, i.e., the electron beam with finite emittance and energy spread. The resultant phase-space density can be computed as a function of various variables: photon energy, K value, and phase-space coordinates. For details of numerical implementation of the Wigner function, refer to [6].

Energy Dependence

The phase-space density is calculated as a function the photon energy with other conditions being fixed. In the case of undulator radiation, the target harmonic number should be also specified.

K Dependence (available only for undulators)

The phase-space density at a specific harmonic is calculated as a function of the undulator K value. Note that the photon energy is roughly optimized to give the maximum phase-space density according to respective K values. If the calculation is done on-axis $(x=y=x'=y'=0)$, the resultant data is comparable to “Brilliance at Peak Energy” or “Brilliance Curve” under “Simplified Calculation” (see section 4.6.3), but based on a more rigorous method based on the Wigner function.

Brilliance Curve (available only for undulators)

Similar to “K Dependence” done on-axis, but the harmonic number is automatically selected to maximize the brilliance.

Phase-Space Profile

The distribution of the phase-space density is calculated as a function of the phase-space coordinate variables: *x, y, x'*, and *y'*. Four types of calculation conditions are available as follows:

(1) X-X' Plane (Sliced)
(2) X-X' Plane (Projected)
(3) Y-Y' Plane (Sliced)
(4) Y-Y' Plane (Projected)
(5) (X,X',Y,Y') Space

The first two denote the distribution on the horizontal phase space (*x, x'*). The difference is that (1) denotes the phase-space density at a fixed (sliced) vertical coordinate (y_{fix}, y'_{fix}), while (2) denotes the distribution projected on (*x, x'*), obtained by integrating over (*y, y'*). The next two (3) and (4) are the same as (1) and (2) but the roles of the horizontal and vertical axes are swapped.

The last one (5) denotes the distribution on the 4-D space (*x, y, x', y'*), the data of which is calculated on the 4-D grid points. Note that the correlation coefficient (see next section) of the Wigner function is recorded at head of the output file.

Properties Computed only in the Fixed Point Calculation

In addition to the phase-space density, two important properties related to the Wigner function method are available: decoupling factor and degree of spatial coherence. Note that these two can be computed only when the Fixed Point Calculation option is selected.

A) Decoupling Factor

In most cases, especially when the electron beam emittance is not too small compared to the optical emittance at the target wavelength, the phase-space density and thus the Wigner function can be decoupled to two functions W_h and W_v that denote the distributions in the horizontal and vertical phase spaces defined as

$$W_h = \iint W(x,y,x',y')dydy' \,, W_v = \iint W(x,y,x',y')dxdx'$$

Then, the Wigner function *W* can be substituted by $W_d = W_h W_v/F$, where *F* is the total photon flux, and the numerical cost for evaluation of the phase-space density is significantly reduced. In order to evaluate the similarity of the two functions *W* and W_d and to examine if the above discussions are valid under a specific condition, the decoupling factor κ has been introduced, which is defined as

$$\kappa = \frac{\langle W_d W \rangle}{\sqrt{\langle W_d^2 \rangle \langle W^2 \rangle}},$$

where <*f*> denotes the average of the function *f* over the range of interest. This is comparable to what is known as the cross correlation coefficient in signal processing and statistics, which ranges from −1 to +1 and gives us the information of how the two functions *W* and W_d are similar to each other. Namely, the two functions are completely similar, if κ is equal to +1.

B) Degree of Spatial Coherence

The degree of spatial coherence ξ in SPECTRA is defined as

$$\zeta = \left(\frac{\lambda}{F}\right)^2 \iint W^2(\boldsymbol{r}, \boldsymbol{r}')d\boldsymbol{r}d\boldsymbol{r}',$$

which is actually a spatial average of the degree of spatial coherence $\mu^2(r_1,r_2)$ usually calculated at two different points r_1 and r_2. This is to avoid the complexity of expressing the function by two coordinate variables. Using the two functions for decoupling the Wigner function, we can also define the degree of spatial coherence in the horizontal or vertical direction as follows.

$$\zeta_x = \frac{\lambda}{F^2} \iint {W_h}^2(x, x')dxdx', \zeta_y = \frac{\lambda}{F^2} \iint {W_v}^2(y, y')dydy',$$

Note that the above properties, κ, ξ, ξ_x, ξ_y are roughly computed by a simple summation of quadratic forms of Wigner functions computed at a number of grid points specified by the user, and the accuracy of integration is not checked. The user is required to specify the range and number of mesh that are sufficiently wide and large to obtain a reliable result. One solution is to first check the profile of the Wigner function in the phase space, then specify these parameters.

4.3.2. Spatial Profile

In addition to the phase-space density based on the Wigner function described above, the spatial profile of the photon density, i.e., the spatial flux density can be computed at the source point. This may be useful when discussing the profile of the photon beam after focusing components in the SR beamline. To be more specific, the spatial profile computed with option reproduces the photon beam profile after the 1:1 focusing mirror.

4.4. Classification by Other Conditions and Procedures

In addition to the classifications described above, there exist a number of important classifications by other conditions that should be addressed.

4.4.1. Observation Scheme for Spatial Dependence

When “Spatial Dependence” is chosen, the user is requested to specify the method to move the observation point. Three options are available: Along Axis, Cartesian Mesh, and Cylindrical Mesh.

Along Axis

The observation position is moved along the horizontal (x) or vertical (y) axis as shown in Figure 4.2 (a). In this case, two output files are created, which correspond to the two axes.

Cartesian Mesh

The observation position is moved in a rectangular area determined by the observation range (x_{max}, etc) as shown in Figure 4.2 (a).

Cylindrical Mesh

The observation position is moved in a sectoral area determined by the observation range (r_{max}, etc) as shown in Figure 4.2 (b).

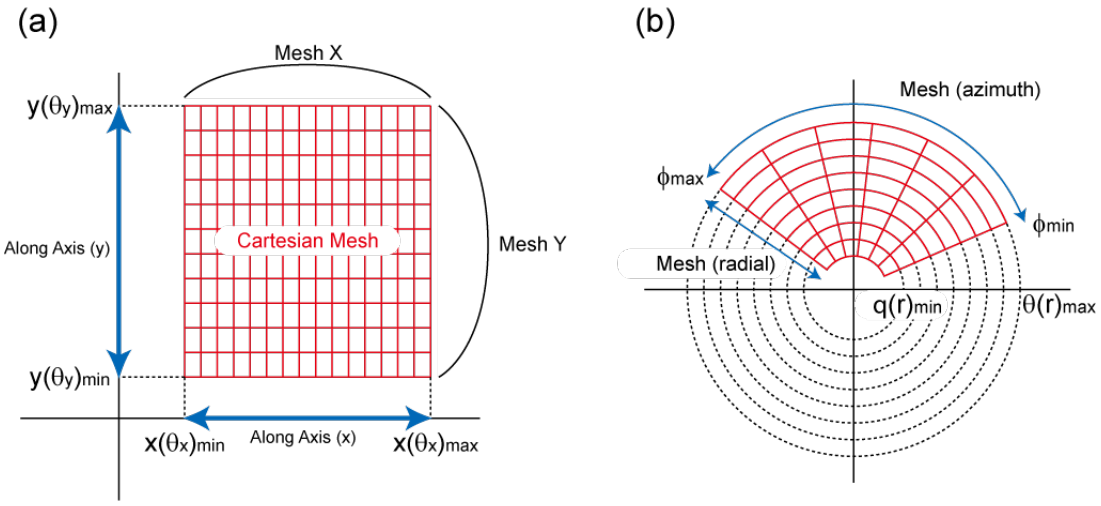


Figure 4.1 Meanings of the observation position in [Along Axis] and [Cartesian Mesh] (a) and [Cylindrical Mesh] (b).

4.4.2. Slit Shape for Partial Flux or Partial Power

In order to calculate the partial flux or partial power, the user is required to specify the dimension and shape of the slit which is assumed to be placed in front of the observation point. Two types of slit shape are accepted: rectangular and circular as shown in Figure 4.1.

"Rectangular Slit" denotes the rectangular-shaped slit with the width of Δx and height of Δy as shown in Figure 4.1 (a), while "Circular Slit" denotes the circular slit or doughnut-shaped slit as shown in Figure 4.1 (b).

The parameters r_1 and r_2 specifies the radii defining the region through which the photon beam passes. If the parameter r_1 is set to 0, the slit reduces to a simple circular slit. The parameters $\Delta\theta_x$, $\Delta\theta_y$, θ_1 and

θ_2 are angles that correspond to Δx, Δy, r_1 and r_2, respectively. To be more specific, $\Delta\theta_x = \Delta x/Z$ and similar expressions for other parameters, where Z is the distance from the SR source to the slit.

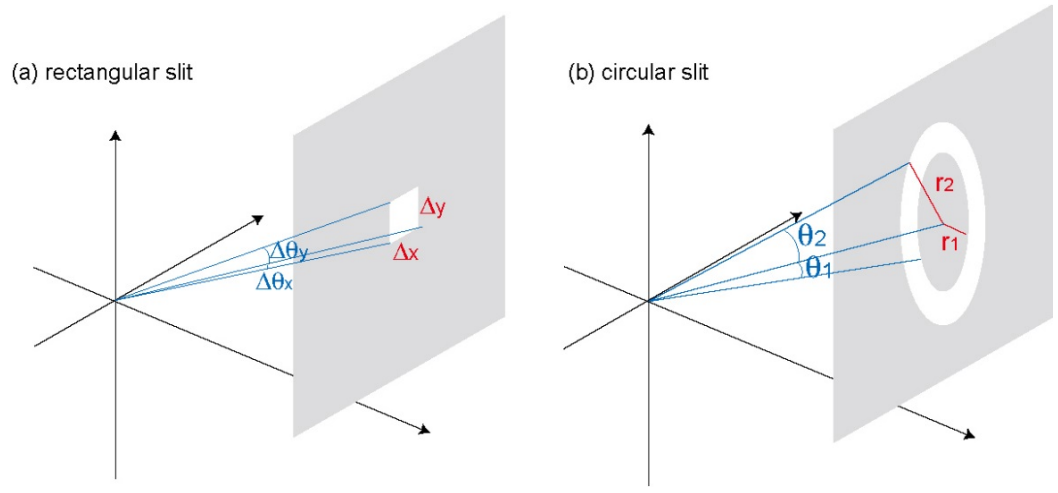


Figure 4.2 Schematic illustration of the (a) rectangular slit and (b) circular slit.

4.4.3. Simplified Calculation

In SR computation, most of the numerical cost is usually coming from the convolution integral, i.e., the convolution of the distribution function of radiation emitted from a single electron with that of the electron beam. If we assume that the SR is a Gaussian beam, it is easy to roughly estimate the light source performances of SR, such as the brilliance, on-axis flux density, source size and angular divergence without actually doing the convolution. Such a simplification is applied when "Brilliance at Peak Energy", "Brilliance Curve", or "Characteristics" is chosen as the main output item.

4.4.4. Flux at Fixed or Peak Energy

When "K Dependence" is chosen from the main menu and "Angular Flux Density" or "Partial Flux" is selected as the main output item, we have two options concerning the setting of the photon energy. One is to fix the photon energy at a certain value specified by the user, which is available by selecting [Flux at Fixed Energy] submenu. The other is to optimize the photon energy at each K value so that the photon flux is maximized, which is available by [Flux at Peak Energy]. In the latter option, *SPECTRA* automatically looks for the optimum energy (peak energy), which is recorded in the output file.

In terms of the practical situation in the SR beamline, the undulator gap is varied to change the fundamental energy in both calculation options, while the monochromator angle is fixed in the "Fixed Energy"case and varied in the "Peak Energy" case to follow the variation of the fundamental energy.

4.4.5. Coherent Radiation

All the calculations under the [Coherent Radiation] category are performed with the temporal and spatial coherence taken into account. Note that the spontaneous radiation is not considered in this option. As a

result, if the bunch length (σ_z, refer to section 5.1) is much longer than the target wavelength, the photon flux and radiation power becomes 0. So the user is requested to carefully check the bunch length and the target wavelength.

As in the case of spontaneous radiation, we need to perform the convolution with the electron beam to accurately evaluate the SR characteristics. The temporal convolution is easily done just by multiplying the bunch-factor spectrum (Fourier transform of the bunch profile of the electron beam). On the other hand, the spatial convolution is quite time-consuming because 4-fold integral in the 4-D phase space spanned by (*x, y, x', y'*) is required, if no approximation is made. In *SPECTRA*, a numerical method is implemented to reduce the computation time under an assumption that the electron beam spatial profile is a slowly varying function of the longitudinal coordinate, which is in most cases valid.

4.5. Other Main Output Items Available

In addition to those mentioned in section 4.2.3, there exist a number of output items available for the main output item as explained in this section.

4.5.1. Items Evaluated by the Simplified Calculation

The output items of calculation type with one of the following main items are evaluated by the "Simplified Calculation" scheme explained in section 4.4.3. Thus the user needs to note that they are just approximated values and maybe less accurate compared to others based on a rigorous numerical computation.

Brilliance at Peak Energy

The brilliance, total flux, etc. are calculated as functions of the peak energy at each harmonic. In addition, the total radiation power and on-axis angular power density are also calculated to indicate the performance of undulator as a SR source. This calculation is convenient to create a graphical plot that shows the performances of various SR sources.

Characteristics

Various characteristics of SR, including the source size and angular divergence, are calculated. Note that the output items depend on the type of the SR source.

Brilliance Curve

SPECTRA looks for the maximum values of the brilliance, flux density and total flux, among the possible harmonic numbers at a given photon energy, and repeat it for different photon energies to create a curve that shows the best performance in the specified energy region. In addition, the coherent fractions in the horizontal and vertical directions are also calculated.

4.5.2. Radiation Field by a Single Electron

The calculation with one of the following main items is done with an assumption that a single electron is injected in the SR source.

Time Dependence

The electric field of SR is calculated as a function of observer's time, which is measured in the laboratory frame but not in the rest frame of electron. Both the vertical and horizontal components of the electric field vector are calculated.

Complex Amplitude Spatial Profile

The complex amplitude, which is obtained by a temporal Fourier transform of the electric field of radiation, is calculated as a function of the transverse observation position. The real and imaginary parts of the complex amplitude are calculated for both the horizontal and vertical polarization components.

4.6. Output Items in Individual Calculation Types

The output items available in the individual calculation types described so far are summarized in Table 4.2 ~ 4.5, for typical “Dependence” and main output items.

Table 4.2 Output items available in Energy Dependence category.

Output Item	Main Output Item				
	Angular Flux Density	Spatial Flux Density	Partical Flux	Total Flux	Characteristics
Angular Flux Density	✓				✓
Spatial Flux Density		✓			
GA. Brilliance	✓				✓
Partical Flux			✓		
Total Flux				✓	
Flux(/eV)					✓
Integrated Flux					✓
Integrated Power					✓
Horizontal Size					✓
Vertical Size					✓
Horizontal Divergence					✓
Vertical Divergence					
PL (s1/s0)	✓	✓	✓		
PC(s3/s0)	✓	✓	✓		
PL45(s2/s0)	✓	✓	✓		
1-|PL|	✓	✓	✓		

Table 4.3 Output items available in Spatial Dependence category.

Output Item	Main Output Item			
	Angular Flux Density	Spatial Flux Density	Angular Power Density	Spatial Power Density
Angular Flux Density	✓			
Spatial Flux Density		✓		
PL (s1/s0)	✓	✓		
PC(s3/s0)	✓	✓		
PL45(s2/s0)	✓	✓		
1-|PL|	✓	✓		
Angular Power Density			✓	
Spatial Power Density				✓

Table 4.4 Output items available in K Dependence category (1).

Output Item	Main Output Item					
	Angular Flux Density		Partical Flux		Angular Power Density	Partial Power
	Fixed Energy	Peak Energy	Fixed Energy	Peak Energy		
Peak Energy		✓		✓		
Angular Flux Density	✓	✓				
GA. Brilliance	✓	✓				
Partical Flux			✓	✓		
PL (s1/s0)	✓	✓	✓	✓		
PC(s3/s0)	✓	✓	✓	✓		
PL45(s2/s0)	✓	✓	✓	✓		
1-|PL|	✓	✓	✓	✓		
Angular Power Density					✓	
Partical Power						✓

Table 4.5 Output items available in K Dependence category (2).

Output Item	Main Output Item		
	Brilliance at Peak Energy	Brilliance Curve	Characteristics
Angular Flux Density	✓	✓	
GA. Brilliance	✓	✓	
Total Flux	✓	✓	
Total Power	✓		
Horizontal Coherent Fraction		✓	
Vertical Coherent Fraction		✓	
Narutal Size			✓
Natural Divergence			✓
Horizontal Size			✓
Vertical Size			✓
Horizontal Divergence			✓
Vertical Divergence			✓
Coherent Flux			✓
Coherent Power			✓

4.7. Abbreviations and Their Meanings in the Output File

In the output file that saves the calculation results, a line composed of abbreviations to denote the SR characteristics and other related quantities is printed at the top of the file. The meanings of these abbreviations are summarized in Table 4.6 together with units used in the output file.

Table 4.6 Abbreviations to denote SR characteristics and related quantities used in the output file.

Abbreviation	Meaning	Unit
`1-|PL|`	Fraction of photons that are not linearly polarized	-
`Brilliance`	Phase-space density based on the Wigner function	photons/sec/mm^2 /mrad^2/0.1%b.w.
`Coh.Flux`	Coherent flux	photons/sec/0.1%b.w.
`CohFrac.x,y`	Coherent fraction in the horizontal or vertical direction	-
`Coh.Power`	Coherent power	W
`Correlation`	Correlation coefficient of the Wigner function	-
`Div.x,y`	Effective source divergence in x and y axes	rad
`E.Field.x,y`	Electric field in x and y axes	V/m
`Energy`	Photon energy	eV
`F.Density`	Spatial or angular flux density	photons/sec/0.1%b.w./mm^2 or /mrad^2
`Filtering`	Filtered power	same as the unit before filtering
`Flux`	Total or partial flux	photons/sec/0.1%b.w.
`Flux.eV`	Total flux in 1-eV bandwidth	photons/sec/eV
`GA.Brill.`	Brilliance evaluated by Gaussian approximation	photons/sec/mm^2 /mrad^2/0.1%b.w.
`Gap`	Magnet gap of an ID	-
`Harm.x,y`	Resolved power density at the target harmonic with horizontally or vertically polarized state	kW/mrad^2
`Horiz.Dens`	Flux density with horizontally polarized state	-
`I_Flux`	Integrated flux	photons/sec
`ImField.x,y`	Imaginary part of complex amplitude of radiation field	V.sec/m
`I_Power`	Integrated power	kW
`K_Value`	K value of an ID	-
`Kx,Ky`	K values of an ID in x and y axes	-
`Nat.Div.`	Natural angular divergence	rad

Abbreviation	Meaning	Unit
Nat.Size	Natural source size	m
Observer-Time	Observer's time	fsec
P.Density	Spatial or angular power density	kW/mm2 or kW/mrad2
P.Energy	Peak photon energy	eV
Prj.Brill.	Projected phase-space density on the horizontal or vertical phase space	photons/sec/mm /mrad/0.1%b.w.
Power	Partial power	kW
PC	Degree of circular polarization, s3/s0	-
PL	Degree of linear polarization, s1/s0	-
PL45	Degree of 45-deg. linear polarization, s2/s0	-
phi	Azimuth angle of observation	degree
r	Radial position of observation	mm
ReField.x,y	Real part of complex amplitude of radiation field	V.sec/m
Size.x,y	Effective source size in x and y axes	m
theta	Radial angle of observation	rad
theta_x,y	Observation angles in x and y axes	rad
Tot.Power	Total power	kW
x,y	Observation positions in x and y axes	mm
X,Y	Observation positions at the source point	mm
X',Y'	Observation angles at the source point	mrad
Vert.Dens	Flux density of vertically polarized component	-

5. Accelerator Specification

In this chapter, instructions to manipulate the parameters specifying the accelerator performance such as the electron energy, beam current, emittance and twiss parameters, are presented. After opening a *SPECTRA* parameter file, all the parameters related to the accelerator performance are indicated in the tabbed GUI panel that appears in a group box named [Accelerator Specification] located on the top of the main GUI window.

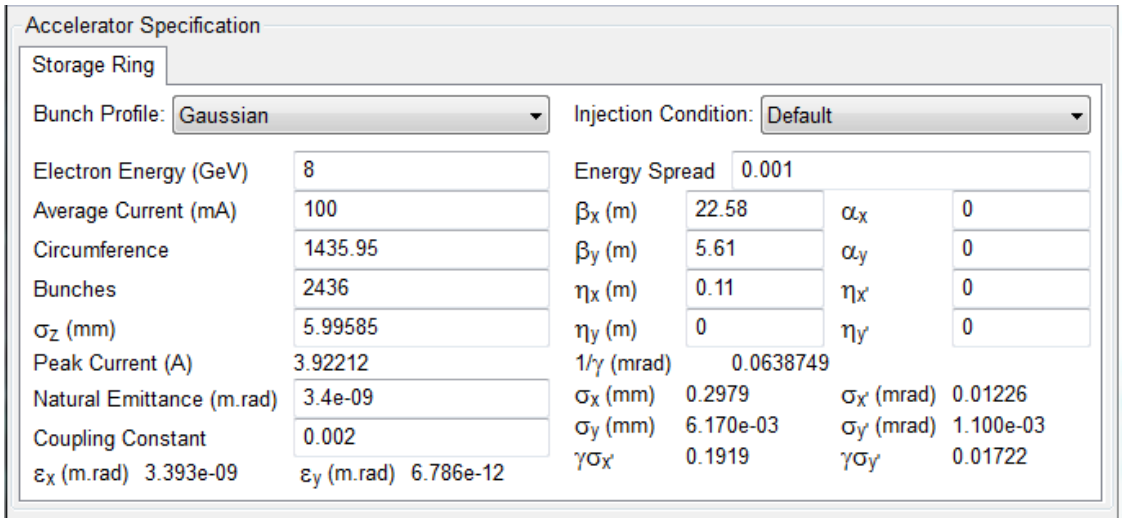


Figure 5.1 GUI window for configuration of [Accelerator Specification]. [Storage Ring] is selected as the accelerator type in this figure.

5.1. Description of Parameters

Figure 5.1 shows the GUI panel for the parameters to specify the accelerator performances when [Storage Ring] has been chosen as the accelerator type (refer to section 5.2). The meanings and units of the parameters are summarized in Table 5.1.

Table 5.1 Descriptions of parameters in the [Accelerator Specification] GUI panel.

Notation	Meaning	Unit	Remarks
Electron Energy	Energy of the electron beam	GeV	
Average Current	Average current of the electron beam	mA	Not editable in Linac (automatically calculated)
Pulses/sec	Electron beam repetition rate	1/sec	Not available in Storage Ring
Bunch Charge	Total charge in a single bunch	nC	
Circumference	Circumference of the storage ring	m	Not available in Linac
σ_z	Bunch length (r.m.s.)	mm	

Notation	Meaning	Unit	Remarks
Peak Current	Peak current of the electron beam	A	
Natural Emittance	Natural emittance of the electron beam	m.rad	
Coupling Constant	Coupling constant ($\varepsilon_y/\varepsilon_x$) of the electron beam	-	
ε_x, ε_y	Horizontal & Vertical emittance	m.rad	
Energy Spread	Energy spread of the electron beam expressed in r.m.s.	-	
β_x, β_y	Betatron function	m	Values at the center of the SR source
α_x, α_y	Lattice function to denote the slope of the phase ellipse of the electron beam	-	
$\eta_{x,y}$,$\eta_{x',y'}$	Dispersion function	m, rad	
$1/\gamma$	Inverse of the Lorentz factor of the electron beam	μrad	
σ_x, σ_y	Electron beam size	μm	
$\sigma_{x'}$, $\sigma_{y'}$	Electron beam divergence	μrad	
$\gamma\sigma_{x'}$, $\gamma\sigma_{y'}$	Electron beam divergence normalized by $1/\gamma$	-	

5.2. Accelerator Type

The accelerator type can be selected by running one of the two submenus in [Configuration]-[Accelerator]-[Accelerator Type]: [Linac] or [Storage Ring]. The difference between the two in *SPECTRA* is the method to specify the average current: it is directly specified by the user in the storage ring, while the pulse repetition rate and bunch charge should be specified in the linac (linear accelerator).

5.3. Bunch Profile

Usually, *SPECTRA* assumes Gaussian profiles for the electron beam distribution functions in the 6-D phase space. If the user needs to specify a customized electron-bunch profile, select [Customized Distribution Function] or [Import Macroparticle Data] from the [Bunch Profile] choice box. In the former option, the projected transverse and longitudinal profiles of the electron beam are required, while in the latter, the macroparticle data in the 6-D phase space are required. For details, refer to sections 5.6 and 5.7. Note that by selecting the customized bunch profile, calculations using the numerical method of "Source Point" (section 4.3) become unavailable.

5.4. Injection Condition

When the SR source contains non-ideal field components such as the dipole field error and field offset as explained in Special Magnet Setup (section 6.5), or [User-Defined] is selected as the SR source type,

the position and slope of the electron averaged over the length of the SR source are not necessarily zero. In such a case, the observer located at the axis of the SR source observes off-axis radiation. In fact, such trajectory errors may be usually corrected by steering magnets in front of the SR source. In other words, the position and slope of the electron beam when injected to the SR source are adjusted to eliminate the trajectory errors.

In order to allow for the trajectory corrections described above in *SPECTRA*, the user is required to specify the injection condition from the options explained in the following sections.

5.4.1. Default

An appropriate injection condition suited to respective SR source is selected. This is usually recommended in most SR sources.

5.4.2. Align Axis at Entrance, Center, Exit

The electron beam axis is adjusted to coincide with that of the SR source. The longitudinal position for adjustment can be selected from the entrance, center, and exit of the SR source.

5.4.3. Custom

In case the user needs to customize the injection condition, select this option. Then [Injection Condition] panel appears as shown in Figure 5.2. Input the initial conditions in position (*x*,*y*) and slope (*x'*,*y'*) at the entrance of the SR source. In order to apply the conditions described above (Default or Align Axis) to be computed by *SPECTRA* and modify the parameters, select one of them and click [Apply Condition] button. The injection parameters are automatically computed and indicated in individual entry boxes.

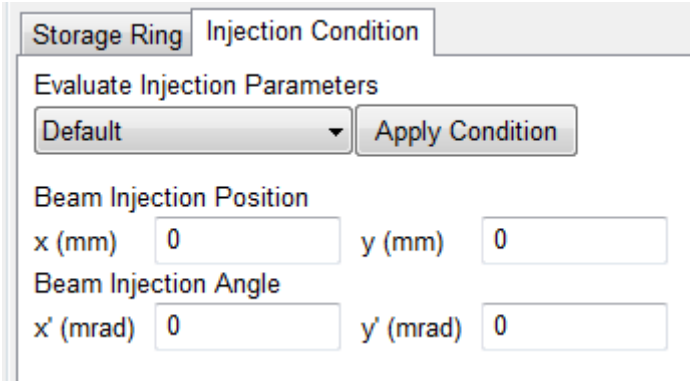


Figure 5.2 GUI window for the configuration of injection conditions.

In order to check if the specified conditions are correct, the user can calculate the electron trajectory and plot it. Refer to section 6.7 for details.

5.5. Plot betatron Functions

In order to check the betatron function as a function of the longitudinal coordinate through the SR sourcce, run [Configuration]-[Accelerator]-[Plot betatron Functions] command after specifying the related parameters and focusing magnets in Light Source Description (chapter 6), and the twiss parameters at the center of the SR source. This command is useful to make sure that the betatron functions are kept appropriate over the length of the SR source, even when focusing magnets are inserted in the SR source.

5.6. Bunch Profile Defined by Customized Distribution Function

If [Customized Distribution Function] is selected as [Bunch Profile], the GUI panel named [Bunch Profile] appears as shown in Figure 4.3, in which the numerical data to specify the bunch profile of the electron beam are manipulated.

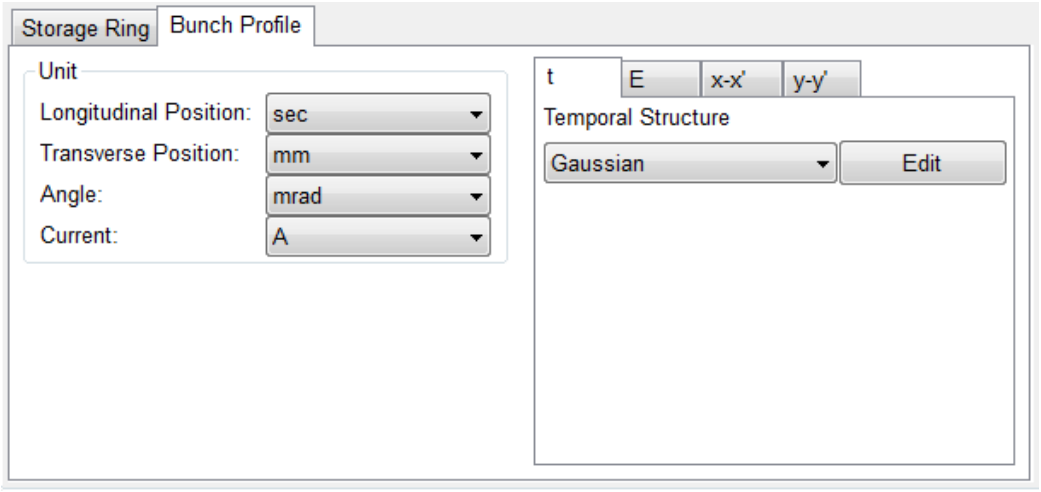


Figure 4.3 GUI panel to specify the customized bunch profile.

Four types of distribution functions should be specified: temporal (t), energy (E), horizontal (x-x') and vertical (y-y'). The first two denote the 1-D functions with a variable of time and energy, while the other two denote the 2-D functions with variables of (x, x') and (y, y'). The user is requested to prepare data files that contain these data sets in ASCII format, as described in sections 5.6.1 and 5.6.2. Then click [Edit] button in one of the tabbed windows titled "t", "E", "x-x", "y-y", run [Import] command, and specify the location of the data file. It is possible to import more than one data for each distribution, in which case the user should select the desired data from the list. It is also possible to select "Gausssian", the default distribution function in *SPECTRA*. The units for the imported data should be selected in the relevant choice box in the [Unit] group box at the left side of the panel.

5.6.1. Format of the 1-D Data

The format of 1-D data set ("t" or "E") should have the format as indicated below (e.g., temporal profile):

```
Time          Current
-5.5E-13      0.07
-4.5E-13      54.3
-3.5E-13      554.5
   (omitted)
1.35E-12      0.8
1.45E-12      0.1
1.55E-12      0.1
```

In the case of energy distribution, the 1st column indicates the energy and the 2nd indicates the intensity. Note that the unit of the intensity is arbitrary. It is automatically normalized to be consistent with the bunch charge.

5.6.2. Format of the 2-D Data

The format of 2-D data set (“x-x” or “y-y”) should have the format as indicated below (e.g., x-x' profile):

```
x      x'     Intensity
-1     -1     0.001
-1     -0.9   0.0011
-1     -0.8   0.0012
   (omitted)
1      0.8    0.0012
1      0.9    0.0011
1      1      0.001
```

The 1st and 2nd column means the grid-like position of the x and x' coordinates, while the 3rd column means the electron beam intensity at the position specified by x and x'. For example, this kind of data is created by a computer program with the source as follows (in C language)

```
for(i = 1; i <= nx; i++){
   for(j = 1; j <= nxp; j++){
      printf("%g %g %g¥n", x[i], xp[j], I[i][j])
   }
}
```

Note that the unit of the intensity is arbitrary as well as the energy distribution data as described above. In order to check if importing the data file is successful, run one of the submenus in [Configuration] - [Accelerator]-[Plot Bunch Profile] to graphically plot the imported data.

5.6.3. Selection of the Unit

After importing the bunch-profile data, the unit for each variable should be selected: mm, m, cm, sec or psec is available for the Longitudinal Position; A or kA is available for the Current, mm or m is available for the Transverse Position; mrad or rad is available for the Angle.

5.7. Particle Data

If [Import Macroparticle Data] is selected as [Bunch Profile], the GUI panel named [Particle Data] appears, in which the numerical data for the macroparticle of the electron beam is manipulated.

In this option, a data file containing information on the macroparticle distribution in the 6-D phase space is required. Such a data file is probably obtained by using other codes to simulate the electron beam dynamics in the accelerator components such as the bunch compressor. *SPECTRA* accepts an ascii file composed of lines containing the coordinates of each macroparticle.

In order to specify the file for the macroparticle data, click [BROWSE] button and specify the location of the file in the file-selection dialog box that pops up. Then a dialog box as shown in Figure 4.4 pops up. In the right, contents of the input data file are shown, while configuration of the input data should be specified in the left.

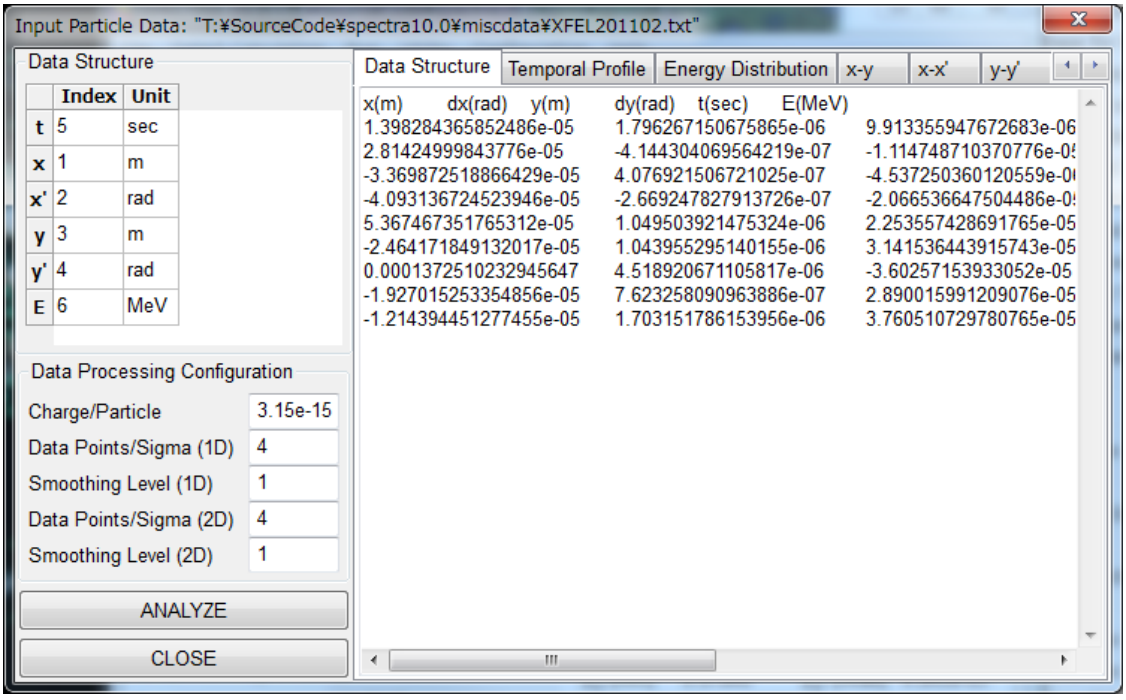


Figure 5.4 GUI window to show the results of analysis on the imported macroparticle distribution.

Each line of the input data file should be composed of 6 coordinates, time (t), position (x,y), angle (x',y') and energy (E). Specify the data arrangement in the [Index] column of the [Data Structure] group box, and the unit of each coordinate in the [Unit] column. For example in Figure 5.4, time (t) is given in the

unit of second and placed at the 5th column, while the horizontal position (x) is given in m and placed at the 1st column.

In order to analyze the input data, edit the parameters in the [Data Processing Configuration] group box, which are used for data processing. “Charge/Particle” refers to the charge per macroparticle. “Data Points/Sigma” specifies the number of data points for visualization and is given as the points per standard deviation of the distribution function. This also defines the data range for averaging: fewer points result in a longer range for averaging and vice versa. “Smoothing Level” determines how the data is smoothed, and higher levels result in smoother data. “1D” or “”2D” means the dimension of data for processing. For example, the bunch temporal profile (beam current given as a function of time) is the 1-D data and thus the parameters for “1D” are used for processing.

After specifying all the parameters, click [ANALYZE] button, then the temporal profile, energy distribution, and profiles in the (x, y) real space, (x, x') phase space and (y, y') phase space, are calculated and shown in the tabbed window with graphical plots. After checking these data sets and related plots, click [CLOSE] button to complete the data import. Note that the data file should not be deleted even after the above processing, because *SPECTRA* saves only the name of the data file in the parameter file, and does not import the data itself. This is in contrast to the other cases such as the data import described in the previous section, or other sections 6.3 and 6.6.4.

6. Light Source Description

In this chapter, instructions to manipulate the parameters describing the SR source such as the magnetic field strength, periodicity, and device length, are presented. After opening a *SPECTRA* parameter file, all the parameters specifying the SR source are shown in the tabbed GUI panel that appears in a group box named [Light Source Description] located on the bottom of the main GUI window. In addition, approximate photon beam characteristics are also indicated.

6.1. Description of Parameters

Figure 6.1 shows an example of the GUI panel for the parameters to describe the SR source. Depending on the SR source type and selected options, up to four tabbed windows appear: the main window for magnetic configurations, Gap-Field Table (6.3), Segmented Undulator (6.4) and Special Magnet Setup (6.5). Refer to the following sections for details.

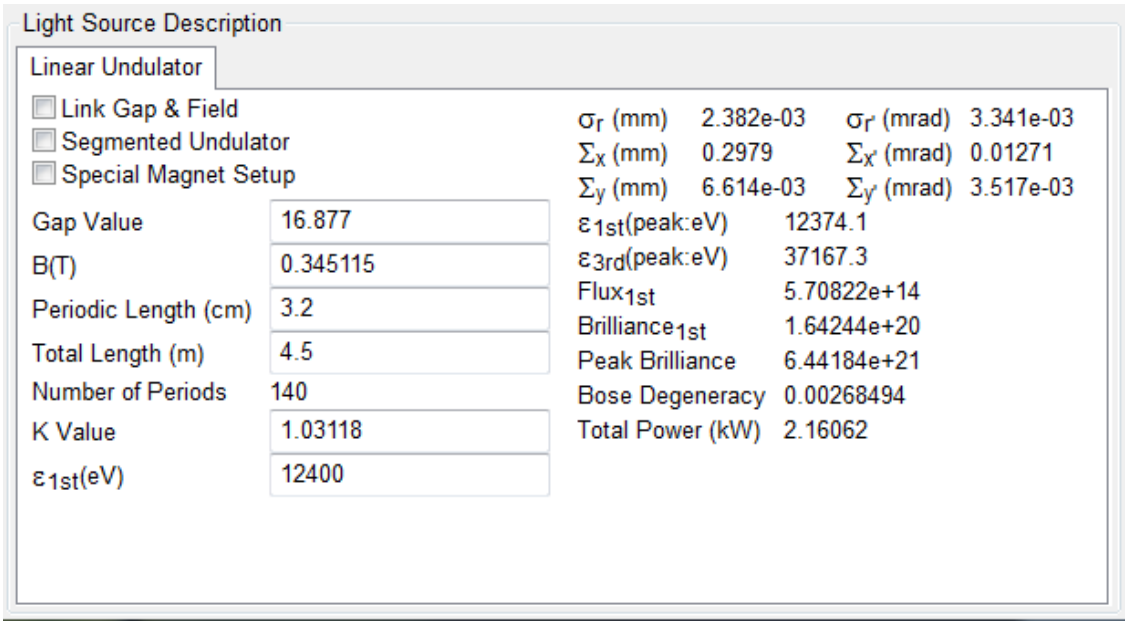


Figure 6.1 GUI window for configuration of [Light Source Description].

6.2. Main Window for Magnetic Configurations

The magnetic configurations for the Built-in SR Source (1.2.1), such as the field strength and periodicity, are indicated in the main panel with a title indicating the source type currently selected. The meanings and units of the parameters in the main panel are summarized in Table 6.1. The configurations for custom SR sources (sections 6.6.2, 6.6.3 and 6.6.4) are different from those in Table 6.1. Refer to sections from Multipole (6.6.2) to User-Defined Source (6.6.4).

Table 6.1 Descriptions of parameters that belong to [Light Source Description]. *The values are approximate ones and available for undulators.

Notation	Meaning	Unit
Gap Value	Gap of the ID	-
Bx,y	Peak magnetic fields in the x and y axes.	T
B	Magnetic field in the principal direction. Peak for IDs and uniform for BM.	T
Radius	Radius of the electron orbit. Available for BM.	m
Periodic Length	Periodic length of the ID	cm
Number of Periods	Number of periods of the ID	-
Total Length	Total length of the ID	m
Kx,y	Horizontal and vertical K Values	-
K	K Value	-
ε1st	Energy of the 1st harmonic	eV
σr,r'	Natural size and divergence of the photon beam at ε1st.	m,rad
*Σx,y, Σx',y'	Effective beam size and divergence of the photon beam at ε1st.	m,rad
*ε1st, 3rd (peak)	peak energy for the 1st and 3rd harmonics	eV
*Flux1st	Total flux at ε1st.	photons/sec /0.1%b.w.
*Brilliance1st	Brilliance at ε1st.	photons/sec/mrad2 /mm2/0.1%b.w.
*Peak Brilliance	Brilliance at ε1st at the peak current of the electron bunch.	photons/sec/mrad2 /mm2/0.1%b.w.
*Degeneracy	Bose degeneracy.	-
Total Power	Total radiation power. Not available for BM.	kW
Critical Energy	Critical energy corresponding to the vertical magnet field. Available for wiggler and BM.	eV
Total Power /Revolution	Total power emitted over the whole ring. Available for BM.	kW
Linear Power Density	Linear power density emitted by the electron beam	kW/mrad

6.3. Gap-Field Table

In general, the magnetic field of a SR source is tuned by changing the gap between the top and bottom magnet arrays. The relation between the field strength and gap value is thus important. *SPECTRA* links the magnetic field with the gap value according to the relation specified by the user. In order to enable this option, tick the [Link Gap & Field] check box. Then, the tabbed window with the title [Gap-Field Table] appears as shown in Figure 6.2.

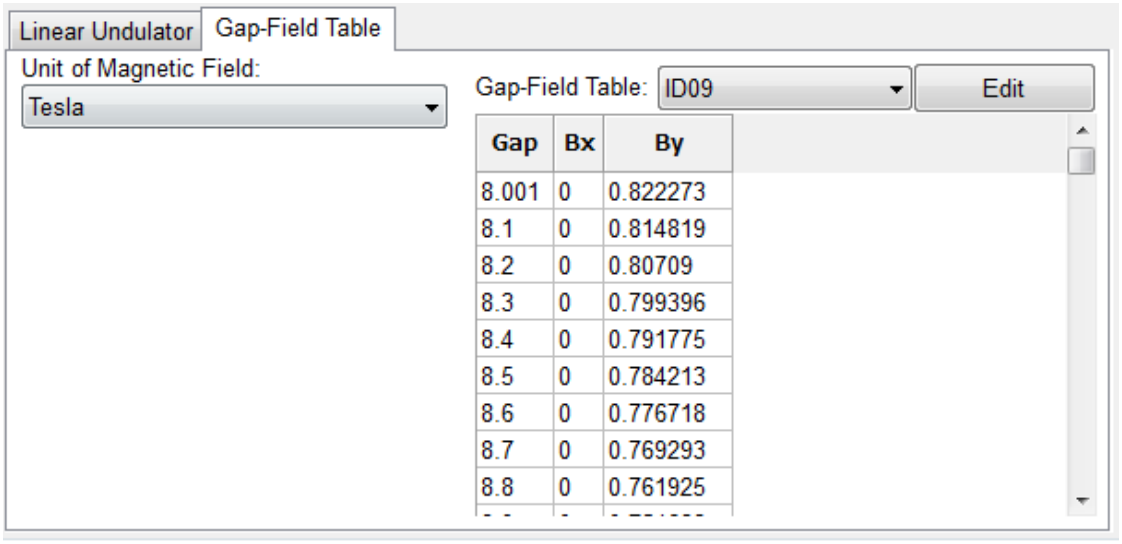


Figure 6.2 Tabbed window that shows the gap-field relation.

The spread sheet shows the relation between the gap and field. Select the desired data from the choice box. In order to import a new table, prepare an ASCII file with the format

```
Gap    Bx     By
50.0   0      0.0284231
48.9   0      0.0312138
47.9   0      0.0339968

     (omitted)

6.26   0      1.11445
6.13   0      1.12545
6.0    0      1.13648
```

The 1st column means the gap value, while the 2nd and 3rd mean the horizontal and vertical magnetic field amplitudes that is used to calculate the K values. Then click [Edit] button and run [Import Gap-Field Table] command. Specify the location of the above file in the file-selection dialog box. The spread-sheet at the right side shows the contents of the imported table. Select the correct unit for the magnetic field from the choice box at the left side.

6.4. Segmented Undulator

Undulators are sometimes divided into several segments. If SR emitted from individual segments is coherently superimposed, the optical characteristics strongly depend on the undulator type and optical phase $\Delta\phi$ (determined by the length of the electron path) between segments. *SPECTRA* is equipped with functions to calculate optical properties of such segmented undulators. Tick [Segmented Undulator] check box in the main GUI panel, then the tabbed panel named [Segmented Undulator] appears as shown in Figure 6.3.

The parameters in the panel are divided into two groups. One is to specify the details and method of segmentation, while the other is to specify the field error due to segmentation.

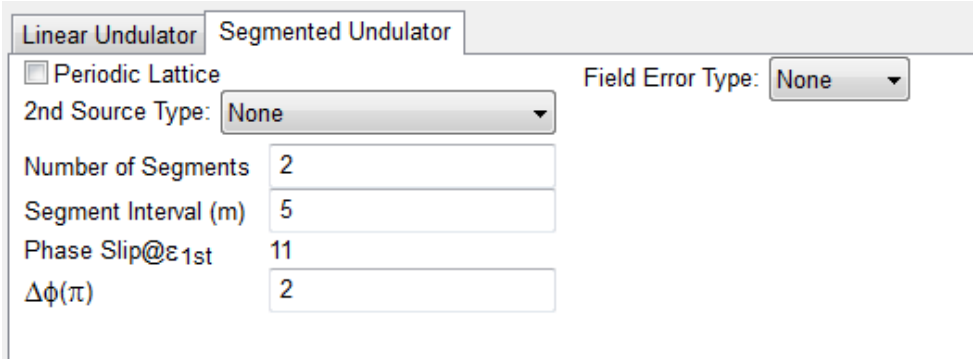


Figure 6.3 GUI panel for configuration of the segmented undulator.

6.4.1. Segmentation Details

In general, $\Delta\phi$ should be set to an integer multiple of 2π to obtain the maximum photon intensity. Contrary to this, there are several schemes to improve optical characteristics of SR that take advantage of undulator segmentation. One is to intentionally introduce a mismatched phase between segments to suppress the higher harmonic intensity [7].

Another application of undulator segmentation is to control the polarization of SR [8]: in this case, an undulator configuration composed of two types of undulator segments is adopted, which is schematically shown in Figure 6.4.

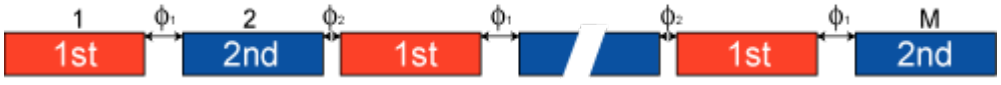


Figure 6.4 Segmented undulator scheme for polarization control.

In *SPECTRA*, several types of undulator segmentation are available ([2nd Source Type]) and the optical phase between segments ([Relative Phase]) can be specified, the details of which are explained in the followings.

2nd Source Type

Type	Meaning
None	The type of all segments and relative phase between them are identical.
Swap Bx and By	Swap Bx and By. The vertical and horizontal fields are swapped in the 2nd source type, i.e., if the 1st type is a conventional linear undulator, then the 2nd type is a vertical undulator.
Flip Bx (By)	Flip Bx (By). Flip the polarity of the horizontal (vertical) field in the 2nd source type, respectively. This makes nothing if the 1st source is a linear undulator, while the helicity of the 2nd source is flipped if the 1st source is a helical (elliptic) undulator.
Custom Setting	Specify the details of each segment Refer to Customizing the Segment (section) for details.

Relative Phase

Notation	Contents
$\Delta\phi$	Optical phase between segments when [None] is selected as [2nd Source Type]
ϕ_1	Optical phase between (*2n-1*)-th and (*2n*)-th segments. (e.g., 1-2, 3-4, ..)
ϕ_2	Optical phase between (*2n*)-th and (*2n+1*)-th segments.(e.g., 2-3, 4-5, ..)

6.4.2. Customizing the Segment

If [Custom Setting] is chosen for the [2nd Source Type], the user is requested to create a data set to specify the details of each undulator segment. In order to create a new data set, click [Edit] button and run [Create New Data Set] command. Then a spreadsheet appears, which has three columns titled as "Type", "N-Ndef.", and "Phase" with the segment number indicated at the 1st column. The meanings of respective columns are summarized as follows. Specify the configurations for each segment.

Column Title	Contents
Type	Specify the type of the undulator. [Default] means the same undulator type as that currently specified in [Configuration]-[Light Source]-[Source Type] menu. For other types, refer to the explanation of "2nd Source Type" in the previous section.
N-Ndef.	Difference in the number of periods from the default value shown in Main Window (section 6.2). If the number of periods is the same as default, 0 should be input here.
Phase	Phase between segments in the unit of π

In order to change the number of segments, run [Add New Segment] command to increase, or [Remove Selected Segment] to remove the segment currently in selection. Note that these commands do not appear when there is no data set stored. Also note that more than one data set can be stored. To do so, click [Edit] button and run [Create New Data Set] command to create a new set, or [Duplicate Data Set] command to copy the current set.

6.4.3. Periodic Lattice

When the number of undulator segments is large and the total length is quite long as in the case of X-ray free electron lasers, focusing magnets are usually installed between undulator segments to keep the betatron function appropriate. In such a case, the betatron function is periodic with a periodic length of the segment interval. In order to specify such a situation, tick the [Periodic Lattice] checkbox, then *SPECTRA* automatically arranges the focusing magnets to realize the lattice.

In this case, the betatron values (β_x, β_y) specified in [Accelerator Specification] are assumed to be those at the undulator center. If non-zero values are specified for the alpha parameters (α_x, α_y), then it is assumed that alpha values at the center of the odd-integer segments are equal to αx, αy, while those of the even-integer segments are equal to $-\alpha_x$, $-\alpha_y$

6.4.4. Specification of Field Errors by Undulator Segmentation

The undulator segmentation can give rise to three intrinsic field errors: K-value Discrepancy, Phase Mismatch, and Kick Errors at the drift section between segments. In order to investigate the impacts of these field errors on the characteristics of SR, *SPECTRA* offers functions to generate a magnetic field distribution containing such field errors. In order to enable the errors due to undulator segmentation, select [Random] or [Custom] in [Field Error Type] choice box located at the right side. In the former case, the field errors are generated by a random number generator with a certain integer as a seed. In the latter case, the user should specify the error at each segment.

Random

The parameters necessary for generate the random field error is listed as follows.

Column	Contents
Random Number Seed	A positive integer as a seed for the random number generator. By scanning this parameter (refer to Scanning a Parameter (2.3) for details), it is possible to repeat the calculations with different error models.
K-value Discrepancy	Maximum error in the K-value discrepancy. To be specific, the K value at the *i*-th segment (K_i) is given by $K_i=K(1+dr_i)$, where dr_i denotes the K-value Discrepancy parameter and uniform random number (form -1 to +1) at the *i*-th segment, respectively.
Phase Mismatch	Maximum phase error in the unit of π.
Kick Error X,Y (G.cm)	Maximum kick error in G.cm.

Custom

In this option, the user should specify the error values at each segment. In order to do so, click [Edit] button and run [Create New Data Set] command to create a new data set. Input any name in the dialog

box that pops up. Then click again [Edit] button and run [Add New Segment] command. Input the segment number you need to add in the dialog box that pops up. You will find 4 or 8 columns according to the 2nd Source Type. The parameters in the 1st to 4th columns have the meanings identical to the [K-value Discrepancy], [Phase Mismatch], and [Kick Error X, Y] parameters in the Random option except that these parameters define the actual error values, but not the amplitude for the random error. The parameters in the 5th to 8th columns, to be enabled if necessary, correspond to the 1st to 4th columns, except that they are for the 2nd source segments (which are thus the even-number segments).

The manipulations of the created data set, such as duplicating and removing, are the same as those described in section 6.4.2. So refer to the explanations in that section.

6.5. Special Magnet Setup

In addition to the options on SR sources described so far, *SPECTRA* offers a number of magnet configurations useful for various purposes such as the focusing effect in the periodic field, magnetic tapering, field offset, and (additional) multipole components. In order to enable these configurations, tick [Special Magnet Setup] checkbox in the main GUI panel to show the tabbed panel named [Special Magnet Setup].

6.5.1. Natural Focusing

It is well known that a periodic magnetic field has a focusing effect on the electron beam in the direction of the magnetic field. In order to enable/disable this effect, tick/untick [Bx/By Natural Focusing] check box. Note that enabling [Bx Natural Focusing] for the linear undulator has no effect because no horizontal field exists. This is effective only for the SR source with the horizontal field component such as the helical and figure-8 undulators.

6.5.2. Tapering

In order to broaden the spectral bandwidth, tapering the magnetic field is effective. The user is required to input the fraction of tapering in m^{-1}. For example, tapering of $0.1m^{-1}$ means that the magnetic field strength varies by 10% over the length of 1 m.

6.5.3. Field Offset

The magnetic field offset can be brought by mis-calibration of the Hall probe or the geomagnetic field, and causes a bend in the electron trajectory. The user is required to input the offset field in T.

6.5.4. Multipole Components

In addition to the main field of the SR source (sinusoidal fields in IDs, uniform field in BMs), the multipole components can be superimposed. Refer to “How to Specify Multipole Components?” (6.6.2) for details.

6.6. Selection of the SR Source Type

The SR source type can be selected by running one of the submenus in [Configurations]-[Light Source]-[Source Type], which are explained in Table 6.2

Table 6.2 Type of SR sources available in *SPECTRA*.

Notation	Explanation	Field Profile
Linear Undulator	Conventional linear undulator for horizontal polarization	Sinusoidal
Vertical Undulator	Undulator with horizontal field for vertical polarization	Sinusoidal
Helical Undulator	Undulator for circular polarization with the horizontal and vertical K values being identical	Sinusoidal
Elliptic Undulator	Undulator for elliptic polarization: the horizontal and vertical K values are not necessarily the same	Sinusoidal
Figure-8 Undulator	Undulator having figure-8 shaped electron orbit, for horizontal polarization and low on-axis heat load	Sinusoidal
Vertical Figure-8 Undulator	Same as figure-8 undulator, but for vertical polarization	Sinusoidal
Multi-Harmonic Undulator	Refer to section 6.6.2	Custom
Wiggler	Conventional wiggler.	Sinusoidal
Elliptic Multipole Wiggler	An elliptic multipole wiggler for elliptic polarization in the high energy region	Sinusoidal
Bending Magnet	Conventional bending magnet	Uniform
Multipole Field	Refer to section 6.6.3	Custom
Field Mapping	Refer to section 6.6.4	Custom
User Defined: Periodic	Refer to section 6.6.5	Custom (but periodic)
User Defined		Custom

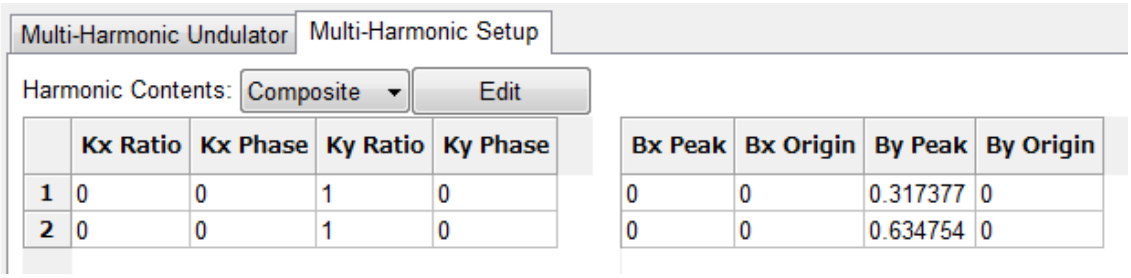
6.6.1. SR Sources with an Ideal Field Profile

In the build-in sources, the magnetic field is assumed to be sinusoidal (undulators and wigglers) or uniform (bending magnet), and calculations with the Far Field Approximation are possible to save the computation time. The difference between the undulator and wiggler is that the photon beam is coherent (undulator) or not (wiggler).

6.6.2. Multi-Harmonic Undulator

“Multi-Harmonic Undulator” is a “semi-customized” undulator, in which the magnetic field distribution is composed of a number of harmonic components. The strength and phase of each harmonic should be defined by the user. Refer to the instruction as follows.

Upon selection of this option as the SR source, a tabbed window named “Multi-Harmonic Setup” appears, as shown in Figure 6.5.



	Kx Ratio	Kx Phase	Ky Ratio	Ky Phase	Bx Peak	Bx Origin	By Peak	By Origin
1	0	0	1	0	0	0	0.317377	0
2	0	0	1	0	0	0	0.634754	0

Figure 6.5 Setup for “Multi-Harmonic” undulator.

In order to specify the configurations of this undulator, the user is first requested to create a data set to define the conditions of individual harmonic components, i.e., the amplitude and origin of the sinusoidal field distribution. In order to do so, click [Edit] button and run [Create New Data Set] command. Enter a desired name in the dialog box that pops up. Then, two spread sheets appear in the left and right side of the window. The numbers indicated at the 1st (left) column of individual rows denote the harmonic numbers. In order to change the maximum harmonic number, click [Edit] button, run [Change Max. Harmonic] and input a desired number to specify the maximum harmonic number.

The field amplitude and origin of the sinusoidal field of the *n*-th harmonic component can be specified by inputting values at each cell of the *n*-th row in the left spread sheet. Input the ratios of the K values in the columns titled “Kx Ratio” and “Ky Ratio”, and phases (in degree) in the columns titled “Kx Phase” and “Ky Phase”. Then the field amplitude and origin are automatically calculated and indicated in the columns titled “Bx/By Peak” and “Bx/By Origin”.

To be specific, let R_n and P_n be the values in the cells at the *n*-th row, 2nd column (titled “Kx Ratio”) and 3rd column (titled “Kx Phase”), respectively. Then the horizontal K value of the *n*-th harmonic component is calculated as

$$K_{xn} = K_x \frac{R_n}{\sqrt{R_1^2 + R_2^2 \cdots + R_N^2}}$$

where *N* is the maximum harmonic number. The horizontal field profile of the *n*-th harmonic component is given as

$$B_{xn}(z) = B_{pn} \sin\left[2\pi\left(\frac{nz}{\lambda_u} + \frac{P_n}{360}\right)\right] = B_{pn} \sin\left[\frac{2\pi n}{\lambda_u}(z - \delta_n)\right]$$

where λ_u is the undulator fundamental period. The parameters B_{pn} and δ_n denote the amplitude and longitudinal origin of the *n*-th harmonic field distribution, that correspond to the K value of K_{xn} and phase shift of P_n. They are also indicated in the corresponding cells in the right sheet, in the unit of Tesla and

mm, respectively. Note that the parameters B_{pn} and δ_n cannot be edited directly. Instead of these parameters, modify R_n and P_n. The configuration for the vertical field can be done in the same manner.

The manipulations of the created data set, such as duplicating and removing, are the same as those described in section 6.4.2. So refer to the explanations in that section.

6.6.3. Multipole Field

Besides the SR sources such as undulators and bending magnets described in the previous sections, the electron can emit radiation when passing through other magnetic devices such as the quadrupole and sextupole magnets. In *SPECTRA*, multipole components up to the decapole can be specified as the SR source, which is available by selecting "Multipole Field" as the SR source type.

How to Specify Multipole Components?

Figure 6.6 shows the GUI panel for configuration of the multipole data.

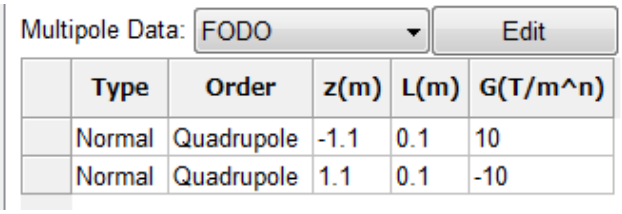


Figure 6.6 GUI panel for configuration of the multipole data.

In order to specify the mulitipole components, click [Edit] button and run [Create New Multipole Data] command. Enter a desired name in the dialog box that pops up. Then, a new spread sheet appears. The meaning of each column is as follows:

Column	Contents
Type	Select [Nomal] or [Skew] as the type of the multipole..
Order	Select the order of the multipole. Up to the decapole is available.
z(m)	Enter the position of the magnet.
L(m)	Enter the effective length of the magnet.
G(T/m^n)	Enter the gradient of the magnet in T and m. If Quadrupole is selected, then the unit is T/m, and so on.

In order to add multipole components, click [Edit] button and run [Add New Magnet] command. Enter the number of magnets to add in the dialog box and click [OK]. Then new rows appear in the spread sheet. Select the type and order of the multipole components, and input the numerical data to specify them.

The manipulations of the created data set, such as duplicating and removing, are the same as those described in section 6.4.2. So refer to the explanations in that section.

6.6.4. Field Mapping

In order to calculate the electron trajectory in the SR source, it is necessary to specify the magnetic field distribution, i.e., the magnetic flux density vector as a function of the 3-dimensional coordinate (***B(r)***). [Field Mapping] is the SR source specified by the numerical data on ***B(r)***.

In order to select this source type, first prepare an ascii file that contains the magnetic field components at 3-dimensional grid points with the format as follows:

```
0.2    0.3    0.5    11     13     421
1.23456e-1    2.3456e-1     3.4557e-1
2.23456e-1    3.3456e-1     6.4557e-1
              (omitted)
4.23456e-1    5.3456e-1     8.4557e-1
2.23456e-1    3.3456e-1     6.4557e-1
```

The 6 numbers in the first line indicate the grid interval in mm and number of grid points along the x, y, and z axes. In the above case, the magnetic field components are given at 11x13x421 grid points with the x, y, and z intervals of 0.2 mm, 0.3 mm, and 0.5 mm, respectively. From the 2nd line, the magnetic field components (Bx, By, Bz) at each grid point are given. The grid point should be moved first in the z direction, next y direction, and finally x direction. For example, such data arrangement will be created by a computer code like this (in C language):

```
for(i = 1; i <= nx; i++){
    for(j = 1; j <= ny; j++){
        for(k = 1; k <= nz; k++){
            printf("%g %g %g¥n", Bx[i][j][k], By[i][j][k], Bz[i][j][k])
        }
    }
}
```

Next, select [Field Mapping] as the SR source type. To show the GUI panel as shown in Figure 6.7. Then click [BROWSE] button and select the data file for the magnetic field distribution with the format described above. In order to check if the data format is correct, run [Configuration]-[Light Source]-[Magnetic Field Distribution]-[Plot Orbit] command and verify the electron trajectory. Before starting

the SR calculation, appropriate units should be selected from the choice boxes at the left of the GUI panel.

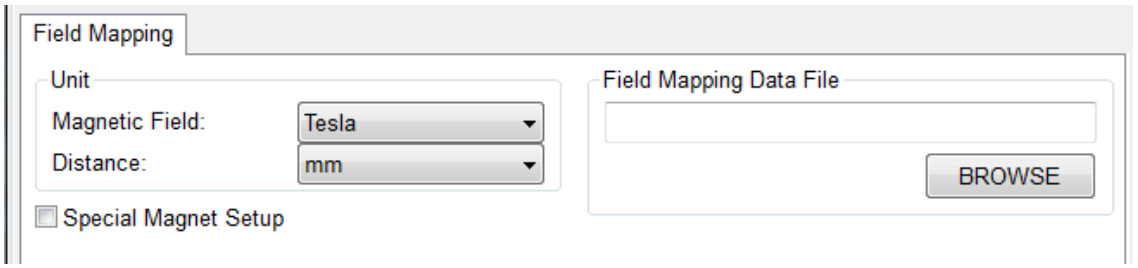


Figure 6.7 GUI panel for configuration of [Field Mappinp] source.

6.6.5. User-Defined Source

In most cases, it is not necessary to specify all the information on the magnetic field distribution to calculate the SR properties. Transverse components of ***B*** measured along the z axis at the origin of the xy plane (Bx(0,0,z), By(0,0,z)) are necessary to approximately calculate the electron trajectory in the SR source. In *SPECTRA*, two SR source types based on this concept are available: [User Defined: Periodic] and [User Defined].

In the former case, the magnetic field is assumed to be periodic. The user is required to import the magnetic field data in a single period and specify the number of periods. This option is useful in the case when the magnetic field distribution is far from a sinusoidal one such as the electromagnet undulators operated in a double-period (or more) mode. In the latter case, the user is required to import the magnetic field data over the whole length, which is probably obtained by the field measurement of the actual device. Note that the Far Field Approximation is not available in the latter case.

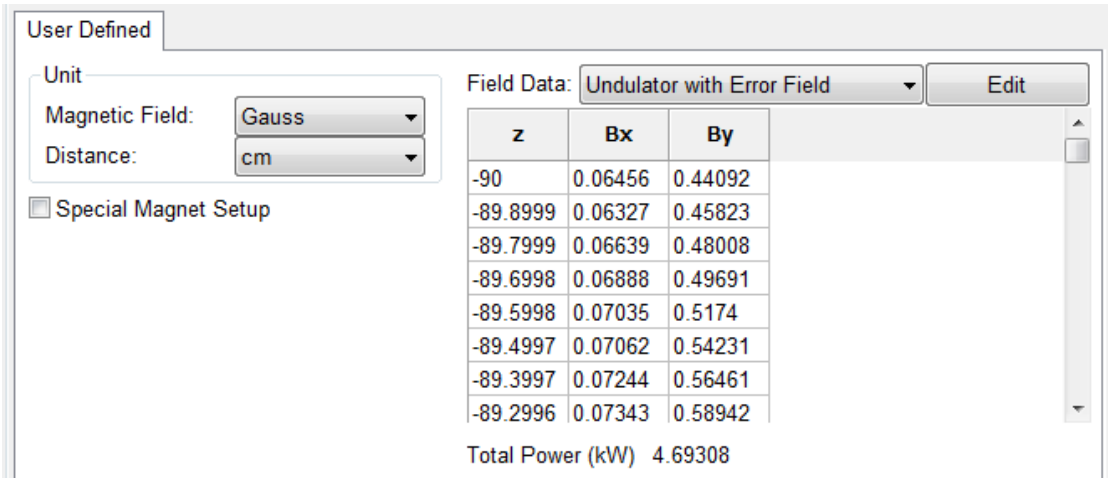


Figure 6.8 GUI panel for configuration common to the [User Defined: Periodic] and [User Defined] sources. In [User Defined: Periodic], several other parameters to specify the periodicity are shown in the left panel.

Figure 6.8 shows the GUI panel for the [User Defined: Periodic] and [User Defined] sources. Select the appropriate unit for the magnetic field (Tesla or Gauss) and longitudinal position (mm, cm, or m). For the [User Defined: Periodic] source, also specify the number of periods.
In order to import the magnetic field data, prepare an ASCII file that contains the field-distribution data:

```
Z              Bx             By
-8.959978e-01 5.174e-05     7.035e-06
-8.949972e-01 5.423e-05     7.062e-06
-8.939967e-01 5.646e-05     7.244e-06
               (omitted)
 8.979989e-01 4.801e-05     6.639e-06
 8.989994e-01 4.582e-05     6.327e-06
 9.000000e-01 4.409e-05     6.456e-06
```

where the 1st column means the position along the longitudinal direction (electron path), the 2nd and 3rd mean the horizontal and vertical magnetic fields, respectively. The title line is not compulsory, and more than one comment lines are accepted. Then click [Edit] button and run [Import Field Data] command. Specify the location of the above file in the file-selection dialog box that pops up. *SPECTRA* loads the data from the specified file and shows it in the spread sheet with the data name (the name of the imported file without suffix) indicated in the choice box. Do not forget to run [File]-[Save] command to save the imported data.

6.7. Checking the Electron Trajectory

If the SR source contains non-ideal magnetic fields, it is recommended to calculate the electron trajectory in the SR source in order to check if the data import in Custom SR Source (1.2.2) is successful and/or configurations in Special Magnet Setup (5.5) are correct. For this purpose, run one of the submenus in [Configuration]-[Light Source]-[Solve Equation of Motion]. Refer to descriptions in Table 8.4.

7. Calculation Configurations

In this chapter, parameters to specify the calculation conditions such as the position of observation and photon energy range are presented, together with the instruction of how to use the other options such as filtering and specification of the numerical accuracy.

7.1. Configuration GUI Window

Upon selection of the calculation type, a GUI window that is independent of the main window pops up, which shows the configurations for calculation. Figure 7.1 shows an example of the window, when [Energy Dependence]-[Angular Flux Density] has been chosen as the calculation type.

The input parameters to specify the calculation conditions are shown in the left side, together with specifications of the photon beam for reference. Besides these parameters, other configurations such as available options, numerical conditions, configurations for the output files, and type of the output items are also indicated in this window.

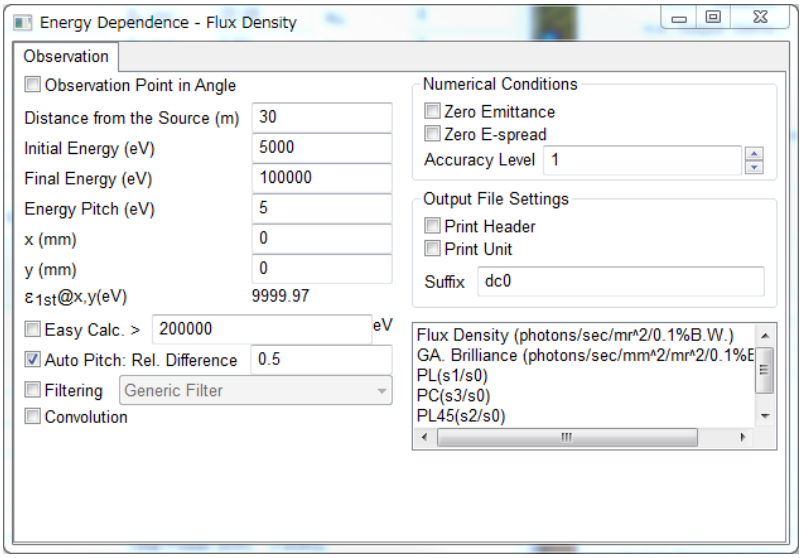


Figure 7.1 GUI window for the calculation configuration ([Energy Dependence]-[Angular Flux Density] is selected in this case).

The input parameters can be divided into several types: energy sampling, harmonic condition, observation position, slit condition, and others. Refer to the following sections for details of them, together with other options related to the numerical algorithm and arrangement of output items.

7.2. Energy Sampling

The parameters for energy sampling refers to those to specify the photon energy range to calculate the spectrum, or target photon energy to calculate the photon flux, and summarized below.

Notation	Meaning	Unit
Initial/Final Energy	Initial/Final photon energies to define the calculation energy range	eV
Mesh (Energy)	Number of calculation points in the energy range.	-
Energy Pitch	Energy pitch to scan the energy. If [Auto Pitch] (section 7.5) option is enabled, this is a maximum value. Available for undulators.	eV
Fixed Energy	Photon energy to be fixed to calculate the photon flux density or Wigner function	eV
Detuning	Normalized photon energy with respect to the target harmonic (available for calculations in “Photon Distribution at Source Point”).	-

7.3. Observation Position

The parameters for observation position refers to those to specify the transverse position of observation, which are summarized below. Refer to Figures 4.1, 4.2, and 7.2 for reference.

Notation	Meaning	Unit
x, y	Observation position in x or y axis	mm
θx, θy	Observation angle in x or y axis	mrad
Minimum/Maximum x, y (θx, θy)	Minimum/Maximum position (angle) in x or y axis, to specify the range of observation in [Along Axis] and [Cartesian Mesh]	mm (mrad)
Minimum/Maximum r (ϕ)	Minimum/Maximum position (angle) to specify the range of observation in in [Cylindrical Mesh]	mm (degree)
Mesh (x, y)	Numbers of grid points in x or y axis	-
Mesh (radial, azimuth)	Number of grid points in r or ϕ axis	-

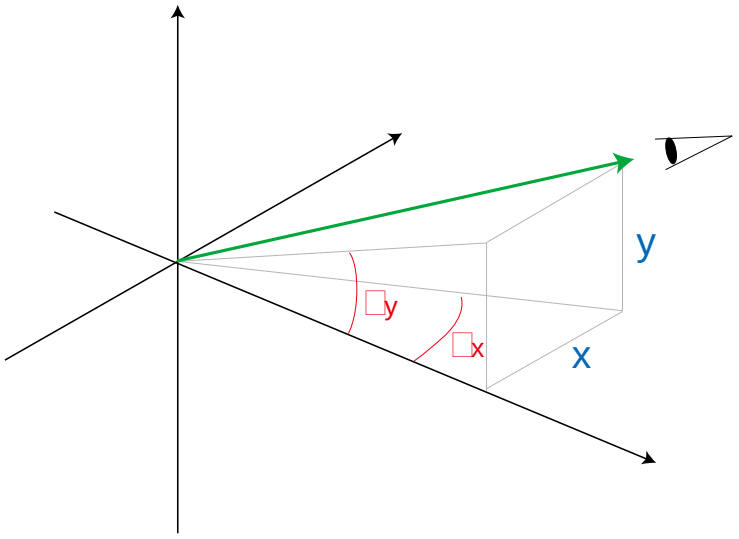


Figure 7.2 Observation of SR at a certain observation position.

7.4. Harmonic Condition

If the selected SR source is of an undulator type, the harmonic number should be considered in several calculation types. The related parameters to specify the harmonic condition are summarized below.

Notation	Meaning
Minimum/Maximum Harmonic	Define the harmonic range.
Target Harmonic	Specify the harmonic number to be fixed.

Note that the harmonic numbers actually available for calculation depend on the numerical method and the type of the SR source. Refer to the followings.

Far Field

In the case of figure-8 and vertical figure-8 undulators, half-odd-integers (0.5, 1.5, 2.5, etc.) as well as integers are available for the harmonic number. For other undulators, only odd integers (1, 3, 5, …) are valid. For example, if Minimum Harmonic is set to 1 and Maximum Harmonic is set to 4, the available harmonic numbers in figure-8 undulators are 1, 1.5, 2, 2.5, 3, 3.5 and 4, while those in other undulators are 3 and 5.

Photon Distribution at Source Point

For figure-8 and vertical figure-8 undulators, the condition is identical to the above. For other undulators, even integers as well as odd integers are available to specify the target harmonic number.

7.5. Slit Condition

The parameters for slit condition refers to those to specify the position and dimension of the slit to be placed in front of the observer.

Notation	Meaning	Unit
x_{slit}, y_{slit}	Slit center positions in x and y axes	mm
θ_{xslit}, θ_{yslit}	Slit center angles in x and y axes	mrad
Δx, Δy	Full width (x) and height (y) of the rectangular slit expressed in length (see Figure 4.1)	mm
$\Delta\theta_x$, $\Delta\theta_y$	Full width (x) and height (y) of the rectangular slit expressed in angle (see Figure 4.1)	mrad
r_1, r_2	Radial positions that specify the circular slit (see Figure 3.3)	mm
$\Delta\theta_1$, $\Delta\theta_2$	Radial angles that specify the circular slit (see Figure 3.3)	mrad

7.6. Other Parameters

Other relevant input parameters are listed below.

Notation	Meaning	Unit	Remarks
Distance from the Source	Distance from the source to the observer, or the slit	m	
Minimum/Maximum K (Ky)	Specify the K-value range		Available in "K Dependence" calculations
Mesh (K Value)	Number of data points		
Mesh (Time)	Number of longitudinal points		
Δx, Δy/2	Half calculation range in x or y axis. The actual calculation range is from -Δx, Δy/2 to Δx, Δy/2	mm	Available in "Complex Amplitude Spatial Profile" (section 4.5.2)
Mesh x, y (Half Range)	Number of grid points in the half range Δx,y/2		

7.7. Photon Beam Specifications

Apart from the input parameters necessary for calculation, several characteristics of radiation are shown for reference, which are listed below.

Notation	Meaning	Unit
ε1st@x,y(slit)	Fundamental energy observed at (x,y) = (θx, θy), or at the slit center (depends on the calculation type). Available for undulators.	eV
Σx,y, (Σx',y')	Effective size (or angular divergence) of the photon beam at [Fixed Energy] at the point of observation. This is an approximate value and may not be valid for undulators, if [Fixed Energy] is far from the harmonic peak energies.	mm (mrad)
Σpx,py (Σpx',py')	Effective size (or angular divergence) of the photon beam in terms of radiation power at the position of observation. Approximate value.	mm (mrad)

7.8. Selecting the Transverse Coordinate

The transverse coordinate (observation position or slit width and height) can be represented either in length (x, y, Δx, Δy) or in angle (θ_x, θ_y, $\Delta\theta_x$, $\Delta\theta_y$). In order to use the latter (in angle), check "Observation Point in Angle" option, which is located at the top of the configuration window if available.

7.9. Easy Calculation

The undulator radiation spectrum consists of several sharp peaks called Harmonic, Harmonic Number. This is a consequence of the fact the undulator radiation is coherent. However, such a peak structure is

smeared in an energy region where high-harmonic radiation is dominant, due to finite emittance of the electron beam, finite angular acceptance of the beamline, and so on. Thus rough estimation of photon flux suffices for most applications in such a high-energy region. The [Easy Calculation] option enables the numerical algorithm for such rough estimation. The user is required to input a photon energy above which this algorithm is applied.

7.10. Auto Pitch

[Auto Pitch] is a numerical method for effective calculation of spectrum composed of sharp peaks such as undulator radiation. The energy pitch would be narrow around the sharp peak and wide at other energies. Refer to Fig. Figure 6.2 for details.

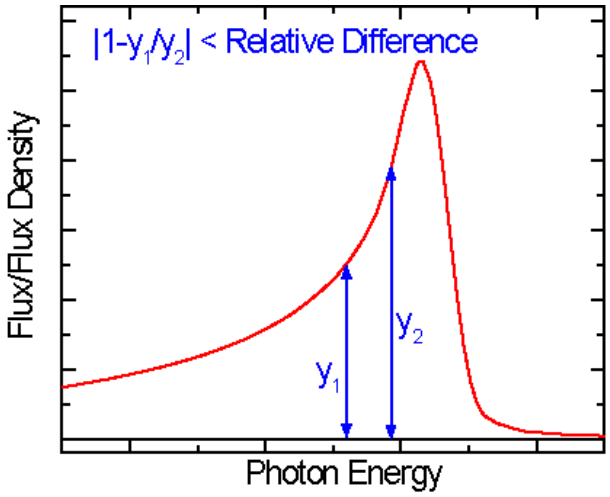


Figure 6.3 Explanation of [Auto Pitch]. When this option is selected, the energy pitch is set automatically so that the value of $|1-y_1/y_2|$ does not exceed the value of [Relative Difference]. Around the energy region where the profile is not steep, the energy pitch would become the maximum value (specified by [Energy Pitch]).

7.11. Filtering

If [Filtering] option is enabled, the characteristics of SR after transmitting an energy filter are calculated in addition to those before the filter. The user should select the filter type from choice box. Three kinds of filters are available: [Generic Filter], [Bandpath Filter], or [Custom Filter].

7.11.1. Generic Filter

[Generic Filter] means a general term for a slab or layer that attenuates the photon-beam intensity, which is usually found in x-ray beamlines of SR facilities, such as a beryllium window for vacuum seal and a layer of air in front of a sample to be irradiated. In *SPECTRA*, any kind of existing elements can be selected as a filter material.

Figure 7.4 shows a configuration window for the generic filter. The user can specify a material and thickness of a filter. The information on the filter material is shown in the [Material Information] group box, and the materials available are listed in the [Material Name] choice box. If the desired material is not found in the list, you can create it. Refer to the following sections in detail.

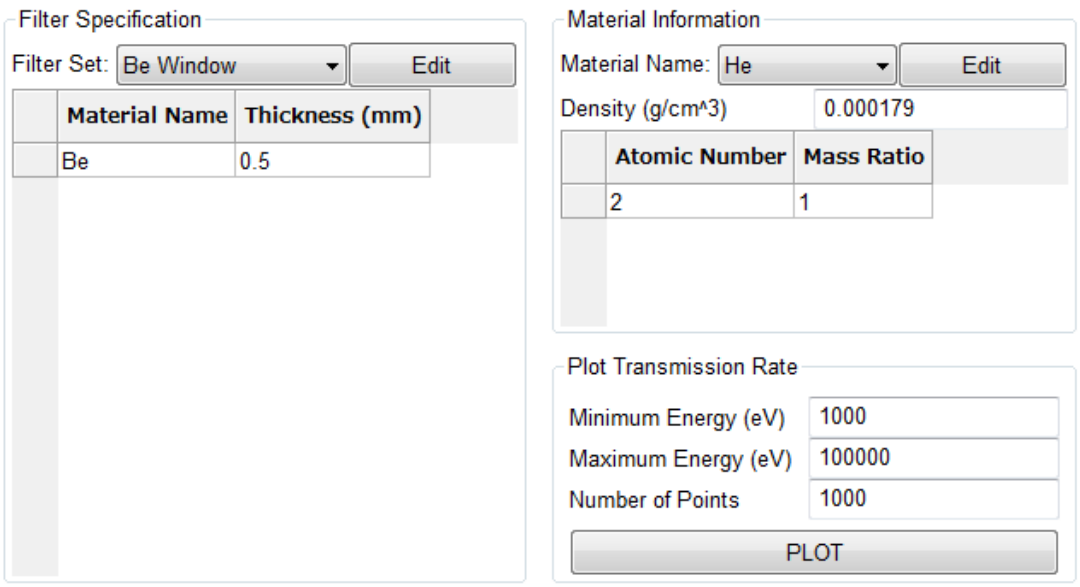


Figure 7.4 Configuration window for the generic filter.

Create a New Filter

In order create a new filter, click [Edit] button in the [Filter Specification] group box and run [Create New Filter] command. Then a new spread sheet with a single row appears. Select the material name and input the thickness of the material in the spread sheet. In order to add new materials, click [Edit] button and run [Add New Material] command. Input the number of materials you need, then new rows appear in the spread sheet for the new material.

Create New Material

In order create a new material for filters, click [Edit] button in the [Material Information] group box and run [Create New Material] command. Input the name of the material in the dialog box that pops up. Input the atomic number and its mass ratio in the spread sheet. In order to add new elements, click [Edit] button and run [Add New Element] command. Input the number of elements you need, then new rows appear in the spread sheet for the new elements.

Plot Transmission Rate

In order to check the transmission rate of the specified filter, input the energy range and number of plotting points in the [Plot Transmission Rate] group box, and then click [Plot] button. A GUI window pops up to show the graphical plot of the transmission rate as a function of the photon energy.

7.11.2. Bandpath Filter

In *SPECTRA*, three types of bandpath filters are available: Gaussian, Lorentzian and Boxcar. For each bandpath filter, the central energy, width (FWHM or full), and maximum transmission rate should be specified. Meanings of these parameters are explained in Figure 7.5.

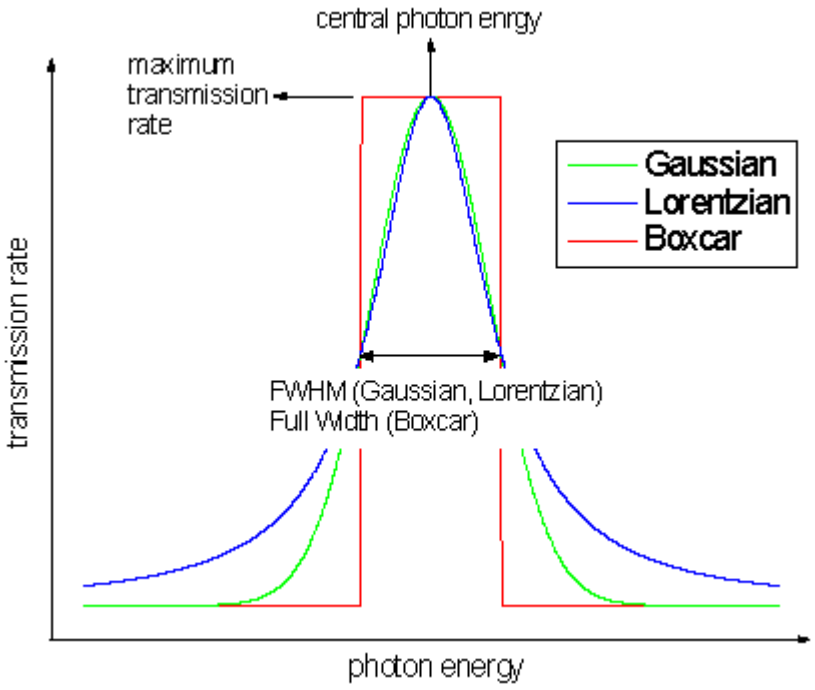


Figure 7.5 Schematic illustration of the three types of bandpath filters available in *SPECTRA*, and parameters that specify the profile of the transmission rate.

7.11.3. Custom Filter

Besides the above two filters, *SPECTRA* accepts a filter that is defined by the user. The input file should have a format indicated below.

```
Energy  Filtering
58071.5  2.261E-4
49680.1  7.972E-4
41482.5  0.0012
  (omitted)
3298.2   0.07375
3123.85  0.06741
2963.5   0.0626
```

In order to import the above file, click [Edit] button and run [Import Transmission Data] command. Specify the location of the above file in the file selection dialog box that pops up. After importing the

data, do not forget to save the parameter file, otherwise the imported data is discarded when opening another parameter file or quitting *SPECTRA*. In order to verify the imported data, click [PLOT Transmission Rate] button to create a graphical plot of the transmission rate.

7.12. Convolution

The energy spectrum measured with a photon detector is in general different from the original spectrum of SR due to a finite energy resolution of the detector, which can be estimated with this option. The resolution of the detector is assumed to be a function of the photon energy with the form

$$[\sigma(\omega)]^2 = a + b\omega$$

where σ is the energy resolution, ω is the photon energy, and *a* and *b* are the parameters dependent on the type of the photon detector and electronic circuit.

In *SPECTRA*, the energy resolution at two different energies should be specified. Then the parameters *a* and *b* are automatically calculated and used for the convolution calculation.

7.13. Numerical Conditions

In the group box titled [Numerical Conditions] located at the right of the [Calculation Configurations] GUI panel, a number of options are available to specify conditions concerning the numerical algorithm. The details are described in the following sections.

7.13.1. Zero Emittance and Energy Spread

The sharp peaks in the spectrum of undulator radiation are broadened by the effects due to the finite emittance and energy spread of the electron beam. In order to estimate SR characteristics without these broadening effects, [Zero Emittance] and/or [Zero Energy Spread] options can be selected instead of substituting 0 for Natural Emittance and Energy Spread parameter (section 5.1), to avoid numerical problems.

7.13.2. Fast Computation Using Swap Files

If the Periodic Lattice option (6.4.3) is enabled, the computation time tends to be very long. This is a consequence of the fact that the convolution of SR with the electron beam requires the 4-dimensional (or 6-dimensional) numerical integration in this case. *SPECTRA* makes use of the Monte Carlo integration method to reduce the computation time. Even so, it is required to repeat many times the calculation of the radiation property from a single electron. A new algorithm that can be applied to reduce the computation time has been developed at SPring-8, in which the total number of numerical operations is reduced drastically. The algorithm is implemented in *SPECTRA*, which is available by enabling this option. Note that a huge memory size is required during the calculation process, and in most cases, swap files are used for that. Specify the maximum size available for such swap files.

7.13.3. Fast Computation

This option is similar to that described in the previous section, but mainly is available for radiation power calculation. In this case, the memory requirement is not severe and thus the swap files are not necessary.

7.13.4. Accuracy Level

In general, a lot of numerical schemes are necessary to calculate SR characteristics, e.g., numerical integration, summation of an infinite series, Fourier transform, and so on. The parameter [Accuracy Level] determines the numerical accuracy of these schemes. It is represented by an integer with a default value of 1. Increasing this number results in a higher accuracy, and vice versa. Needless to say, a higher precision requires a longer computation time.

7.13.5. Numerical Method for Radiation Field

This option determines the numerical algorithm of how to calculate the complex amplitude of the electric field of radiation emitted by an electron moving in the SR source. Select one of the three algorithms: [Fast Fourier Transform], [Direct Integration], [Wiggler Approximation], and [Automatic].

Fast Fourier Transform

Uses a fast Fourier transform (FFT) algorithm to calculate the radiation field. This is always much faster than the [Direct Integration] method and gives correct results in most cases.

Direct Integration

Calculates the radiation field by means of a direct integration. When the radiation field is composed of pulses with a sharp peak as in the case of radiation from IDs with large K values, and edge radiation, the FFT algorithm is sometimes very time-consuming and less accurate. In such a case, this method is more effective.

Wiggler Approximation

Regards the device as a wiggler (i.e., incoherent source). This simplifies the method to calculate the radiation field and gives an approximate result for the flux of SR. Please keep in mind that this method gives incorrect results in the energy region where an undulator spectral profile (composed of sharp peaks) is dominant.

Automatic

SPECTRA automatically judges which algorithm (FFT or Direct Integration) is appropriate in order to reduce the computation time.

Examples

An example to compare the 3 methods described above is shown in Figure 6.5, where spectra for the undulator with error magnetic fields which are calculated with the three different methods are shown. Among them, the [Direct Integration] method takes much longer computation time than the other two.

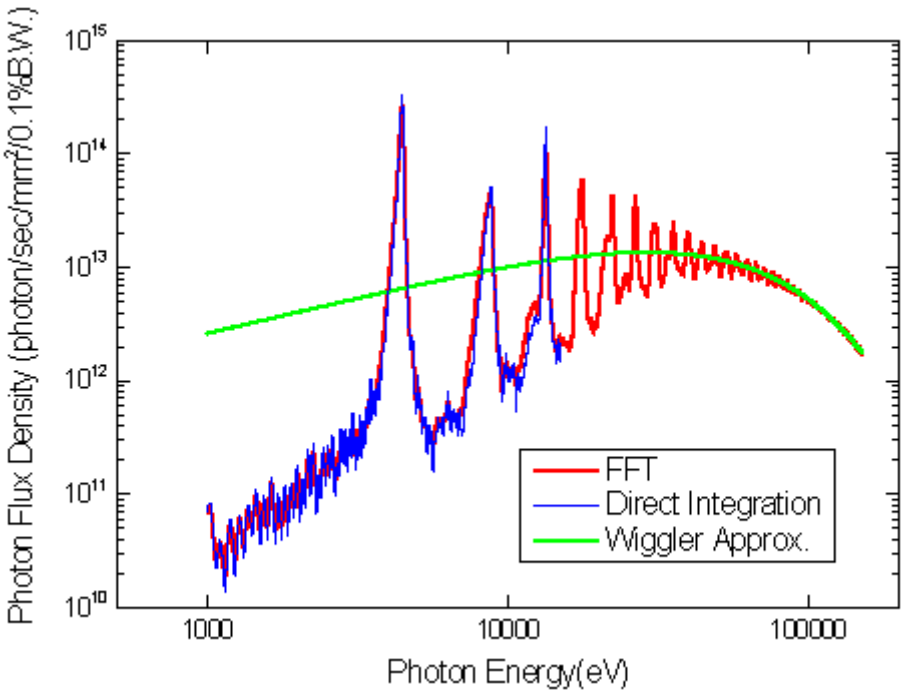


Figure 6.6 Examples to show difference between the 3 numerical methods to calculate the radiation field.

7.14. Options for the Output File

The output file that saves the calculation result can be configured in various ways. Detailed explanations are given below.

7.14.1. Print Header

If this option is enabled, the output file contains a header with information on the calculation conditions, such as the electron energy, emittance, K value, and number of magnetic periods.

7.14.2. Print Unit

If this option is enabled, the output file contains character strings that represent the unit for each item.

7.14.3. Suffix

The name of the output file is composed of a data name and suffix. The data name is specified in the file-selection dialog box that pops up after running, e.g., [Run]-[Start Calculation] command. On the other hand, the suffix should be specified in this option. The number of suffices are dependent on the

type of calculation. For example, the calculation [Spatial Dependence]-[Angular Flux Density]-[Along Axis] needs two suffices for the x and y axes.

Let us consider the case when “[Data Directory]/test” is selected as a data name, and character strings “.dtx” and “dty” are specified as the suffices for x and y axes. Then two files “[Data Directory]/test.dtx” and “[Data Directory]/test.dty” will be created as the output files. It should be noted that several calculation types do not accept the user input for the suffix.

For example, the suffix for [K Dependence]-[Easy Calculation]-[Characteristics] has the format “.dmn”, where “mn” indicates the harmonic number (.d01=1st harmonic, .d03=3rd harmonic), and cannot be defined by the user.

8. Menu Commands

This chapter explains the contents of the menu commands available in *SPECTRA*. Also refer to the related sections for details of each command.

8.1. [File] Menu

Manages the command related to manipulation of the parameter or other files. The submenu commands are summarized in Table 8.1.

Table 8.1 Submenus in [File] menu.

Menu		Action
Create New		Closes the current parameter file and create a new set of parameters.
Open Parameter File		Opens a *SPECTRA* parameter file.
Import Parameter File		Reads parameters in an existing *SPECTRA* parameter file and add the parameters to the current parameters.
Open SPECTRA Output	Data File	Same as the [Import] command in Figure 3.1
	Scan Configu-ration File	Same as the [Import] command in Figure 3.4
	Visualization File	Creates the Animation GUI Window (3.5) with the data file created by the [Save All Data] command.
Save		Saves the current parameters.
Save As		Saves the parameters in another file. Input a new file name in the file-selection dialog box
Initialize Configuration		Initializes the configuration file. Useful in case the behavior of *SPECTRA* looks abnormal.
Exit		Quits *SPECTRA*.

8.2. [Select Calculation] Menu

Selects the type of calculation. Refer to chapter 4 for details.

8.3. [Run] Menu

The submenu commands in [Run] menu are summarized in Table 8.2.

Table 8.2 Submenus in [Run] menu.

Menu	Action
Create Process	Saves the current parameters in the temporary memory and create a calculation process. Refer to Successive Calculations (2.2) for details.
Import Calculation Settings	Loads the file containing the calculation settings which may be created by the [Export …] command below. Also Refer to Successive Calculations (2.2) for details.
Export Calculation Settings	Export the current calculation settings to an external file, which can be loaded again later by running [Import …] command above.
Start Calculation	Starts the calculation. If no processes are created, a single calculation is started using the parameters currently shown in the GUI panels. Otherwise, the calculations in list are performed in series.

8.4. [Open Utility] Menu

The submenu commands in [Open Utility] menu are summarized in Table 8.3.

Table 8.3 Submenus in [Open Utility] menu.

Menu	Action
Simple Plotter	Opens the configuration window to visualize the calculation results (Figure 2.5).
Visualization of Scan Results	Opens the configuration window for Visualization of Scan Calculation (2.5).

8.5. [Configuration] Menu

The submenus in [Configuration] menu are for operation of the parameter sets. Refer to Parameter Set (2.5) for details. Besides the parameter set operation, several commands related to the configuration of the accelerator and light source are summarized in Table 8.4.

8.6. [Help] Menu

Opens this document with a standard PDF viewer installed in your computer. If no standard viewer is found, a warning message is shown.

8.7. [About] Menu

Shows the dialog to show information (version, contact information) on *SPECTRA*.

Table 8.4 Submenus in [Configuration] menu.

Menu		Action
Accelerator	Accelerator Type	Selects the accelerator type (linac or storage ring). Refer to Accelerator Type (5.2) for details.
	Plot betatron Functions	Plot the betatron functions over the SR source. Refer to Plot betatron Functions (5.5) for details.
	Plot Bunch Profile	Plot the distribution functions to specify the bunch profile. Available when [Customized Distribution Function] is selected as the [Bunch Profile] option.
Light Source	Source Type	Selects the type of SR source. Refer to Selection of the SR Source Type (6.6) for details.
	Solve Equation of Motion	Numerically solves the equation of motion of an electron moving in the magnetic field of the SR source. Select one of the submenus to specify the method and items to output the calculation result. If [Save Orbit Data] is selected, the user is required to input a file name to save the calculation result. Otherwise, the results are graphically plotted.

9. Terms on SR

Here, brief explanations on terms on SR used in *SPECTRA* are given. It should be noted that the definitions here are only in the use of *SPECTRA* and other definitions may be given in other applications.

Angular Flux Density

Photons emitted per unit time, bandwidth, and solid angle. The unit used in *SPECTRA* is photons/sec/mrad^2/0.1%B.W, indicating the number of photons emitted per second per 1mrad^2 in 0.1% bandwidth.

Average Flux Density

Flux density of SR transmitting through a slit averaged of the slit area. Given by the partial flux divided by the solid angle or area of the slit. The unit is the same as that used in the Angular Flux Density or Spatial Flux Density.

Angular Power Density

Radiation power emitted into a unit solid angle. The unit used in *SPECTRA* is kW/ mrad^2.

Average Power Density

Power density of SR transmitting through a slit averaged of the slit area. Given by the Partial Power divided by the solid angle or area of the slit. The unit is the same as that used in the Angular Power Density or Spatial Power Density.

Bose Degeneracy

The number of photons in the minimum volume of the 6-D (position: x, y, angle: x', y', energy ω, time t) phase space.

Brilliance

Maximum value of the photon flux density in the 4-D (position: x, y, angle: x', y') phase space. The unit used in *SPECTRA* is photons/sec /mrad^2/mm^2/0.1%B.W.

Coherent Flux

The flux of photons residing within the 4-D phase-space volume defined by full spatial coherence. Refer to [9] for details.

Coherent Power

Portion of the radiated power residing within a 6-D phase-space volume defined by full spatial coherence and a coherence length determined by the undulator period. Refer to [9] for details.

Critical Energy

The photon energy that divides the total-flux spectrum of BM radiation into two parts of equal power. In a more practical meaning, the photon-flux spectrum has its maximum near the critical energy.

Degree of Polarization (PL, PC, PL45)

Degree of polarization of light. There are 3 types of degree of polarization: linear (PL), circular (PC) and 45-degree linear (PL45) polarization. PL = +1(-1) means that the electric vector of the photon beam lies on the horizontal (vertical) plane. PC = +1(-1) means that the electric vector rotates clockwise (counterclockwise). PL45 = +1(-1) means that the electric vector lies on the plane tilted by 45 (135) degree from the horizontal plane.

Harmonic, Harmonic Number

The spectrum of undulator radiation has a sharp peak around an energy corresponding to an integer multiple (=*n*) of a certain energy (fundamental energy) determined by the electron energy, periodic length, and K value(s). SR at such an energy is called *n*-th harmonic and *n* is called a harmonic number.

Integrated Power, Flux

Radiation power and Total Flux of SR integrated from a certain target energy to infinity.

K Value

A dimensionless parameter that denotes the strength of the magnetic field of an ID. Deflection parameter in other words.

Linear Power Density

Power density integrated along the vertical axis.

Natural Size/Divergence, Effective Size/Divergence

Natural size (divergence) is the photon beam size emitted from a single electron (or zero-emittance electron beam) and effective size (divergence) is the photon beam size (divergence) emitted from a finite-emittance electron beam. The effective size (divergence) is given by convolution of the natural size (divergence) with the electron beam size (divergence).

Partial Flux

Photon flux of SR transmitting though a slit. The unit used in *SPECTRA* is photons/sec/0.1%B.W.

Partial Power

Radiation power of SR transmitting through a slit.

Spatial Flux Density

Photons emitted per unit time, bandwidth, and area. The unit used in *SPECTRA* is photons/sec /mm^2/0.1%B.W., indicating the number of photons emitted per second per $1mm^2$ in 0.1% bandwidth.

Spatial Power Density

Radiation power emitted into a unit solid area. The unit used in *SPECTRA* is kW/ mm^2.

Total Flux

Photon flux emitted over the total solid angle (4π). The unit used in *SPECTRA* is photons/sec/0.1%B.W.

Total Power

Power emitted over the total solid angle (4π).

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