#XOP on-line help file: bfield.txt

A program called BFIELD.F is distributed with YAUP.F. BFIELD.F is a standalone module that generates a B-field file for an undulator with a linearly tapered gap in a format acceptable to YAUP. The user must specify the gap GZMIN at Z=Zmin=0 and the amount of gap taper DG=(GZMAX-GZMIN)/GZMIN (either positive or negative). The program interpolates the gap linearly between GZMIN and GZMAX. The field strength dependence is specific to the proposed APS undulators but the user may modify this section of the program according to his/her specific needs. Zero phase errors are assumed. See the file BFIELD.F for more details.

#XOP on-line help file: black_body.txt

================================ BLACK BODY ================================

BLACK_BODY is an widget based graphical interface to calculate the spectum of a black body emitter as a function of the photon energy.

The formulas used can be obtained, for example, from:
David Attwood
Soft X-rays and extreme ultraviolet radiation. Principles and applications
Cambridge University Press, 2000, Pags. 242-246

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
 Black_body input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
  Write Files for XOP/Optics: Saves the current undulator spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files to be used for the other XOP application from Optics menu.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main BLACK_BODY window. Please refer to the information under the HELP button for a complete description of the parameters.
Set Defaults: Sets the default parameters.

Show: Display results. Several options are available
  Plot Results: Makes a plot pf the results
  View Results: Diaplays some numerical information

Help: Shows the BLACK_BODY help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: srio@esrf.fr 2003-01-08

#XOP on-line help file: black_body_par.txt

Description of the input parameters for BLACK_BODY:
==========

TITLE: Information title

TEMPERATURE [K]: The emitter temperature in Kelvin

MIN ENERGY [eV]: Minimum photon energy for the calculated spectrum, in eV.

MAX ENERGY [eV]: Maximum photon energy for the calculated spectrum, in eV.

NUMBER OF POINTS: Number of energy points for the energy spectra

#XOP on-line help file: bm.txt

================================== BM ==================================

BM is an widget based graphical interface to calculate the spectum
of Bending Magnets as a function of the photon energy.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
BM input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Write Files for XOP/Optics: Saves the current undulator spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files to be used for the other XOP application from Optics menu.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main BM window. Please refer to the information under the HELP button for a complete description of the parameters.
Set Defaults: Sets the default parameters.

Show: Display results. Several options are available
Plot energy spectra
Plot angular distribution (all wavelengths)
Plot angular distribution (one wavelength)
Plot (angular,energy) distribution
View numerical values

Help: Shows the BM help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: srio@esrf.fr 2002-06-04

#XOP on-line help file: bm_par.txt

Description of the input parameters for BM:

MACHINE NAME: Information title

B FROM:For selecting B field from either Magnetic radius of the bending magnet or magnetic field.
(The three precedent parameters are related by:
Radius [m] = (10/3) * Energy[GeV] / B[Tesla])

MACHINE RADIUS: The radius of the Bending Magnet in meters.

MAGNETIC FIELD: The magnetic field of the bending magnet in Tesla.

BEAM ENERGY: The electron beam energy in GeV.

BEAM CURRENT: The electron beam current in Ampers.

HORIZ DIV: The horizontal divergence in mrad.

PSI (VERTICAL DIV) FOR ENERGY SPECTRA: For the calculation of the FLux and Power density spectra, different options of Psi can be selected:
Full (integrated in Psi): Spectra are calculated integrated from all space over Psi
At Psi=0: Spectra (pre mrad in Psi) at the center of the beam Psi=0
In [Psi_Min,Psi_max]: Spectra integrated over a given interval in Psi. The values of the interval (Psi_Min and Psi_max) must be entered and also the mumber of points for integration in Psi.

MIN PHOTON ENERGY: Minimum photon energy for the calculated spectrum, in eV.

MAX PHOTON ENERGY: Maximum photon energy for the calculated spectrum, in eV.

NUMBER OF ENERGY POINTS: Number of energy points for the energy spectra

SEPARATION BETWEEN ENERGY POINTS: Two options are available for creating the energy array:
Lin: Energy points are a linear array (constant step)
Log: Energy points are a logarithmic array (step changes as log)

MAX Psi[mrad] FOR ANGULAR PLOTS: Define the maximum value of Psi in mrad to be used when selecting the angular distribution plots, i.e.:
Plot angular distribution (all wavelengths)
Plot angular distribution (one wavelength)

Psi min [mrad]: minimum value of Psi [mrad] for integration. Used in
Plot energy spectra in [Psi_Min,Psi_Max] angular range
Plot (angular,energy) distribution
Use also this entry to place the Psi value to be used when calculating
Plot energy spectra at Psi=Psi_Min

NUMBER OF PSI POINTS: Number of points for Psi integration or for the (angular,energy) mesh distribution. Please note that in the case that an integration over an angular interval [Psi_Min,Psi_Max] is chosen, the accuracy of the result may depends on this number of points in the integration grid.

#XOP on-line help file: crl.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:19 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/crl.pro -----

================================   CRL   ================================

CRL is an widget based graphical interface to calculate the parameters of Compound Refractive Lenses (CRL).

Two kind of calculations are allowed:
i) main parameters (focal distances, gain, acceptance, etc.) (calculated using Refs. 1 & 2)
ii) Pseudo-Ray-Tracing to compute the beam profile at the image plane and the phase-space plot. (calculated using Ref. 2, formulas 9 and 32 for cylindrical and parabolic lenses, respectively).

Reference 1:
A. Snigirev, V. Kohn, I. Snigireva, A. Souvorov and B. Lengeler:
"Focusing High Energy X-rays by Compound Refractive Lenses",
Applied Optics 37 (1998) pp. 653-662)

Reference 2:
P. Elleaume:
Nucl. Instrum. and Meth in Phys. Research A 412 (1998) pp. 483-506

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
CRL input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main CRL window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the "GO CALCULATE" button, CRL starts running. Note that, differently from most of other XOP applications, this "Set Parameters" window is a non-modal window.
Set Defaults: Sets the default parameters.

Help: Shows the CRL help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations with the CRL aplication may also cite the reference mentioned before.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: dabax.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:13 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/dabax.pro -----

================================ DABAX ================================

   DABAX is a widget based graphical interface to visualize and
   process data stored in the DABAX data base.

   This is the main interface that allows to access to the contains
   of the files, makes plots and start processing applications based
   on that files.

   More information about DABAX can be found at the XOP web page
   (select the DABAX entry):
   http://www.esrf.fr/computing/scientific/xop

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
   Download new DABAX file...
        Information on how to add and update files to your DABAX directory.
        It also includes a socket mechanism to automatically download and instal
l
                files.
   Quit: to exit from the program
  Edit:
   DABAX Path: Permits to edit the DABAX path. Dabax path is a
        list of directories (separated by columns ':') that
        define the placed where the DABAX files are located.
        The utility of redefining the DABAX path here is to add
        user-files located in user directories.
  View:
   Refresh File List: refresh main window with DABAX list of files.
   DABAX Path: Displays the current DABAX Path.
   Full File Name: Displays the Full name of the selected DABAX
        file. This is useful when several versions of a file
        with the same name are present in different directories
        in the DABAX path.
  Help:
   DABAX: Displays doc of DABAX interface application (this text).

 COPYRIGHT:
        DABAX belongs to XOP package and it is distributed within XOP.
        PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

 CREDITS:
        Published calculations made with XOP should refer:

          M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
          SPIE proceedings vol. 3448, pp.340-345, 1998.

 LAST MODIFICATION: msr/msr/03-01-10

```
#XOP on-line help file: editor.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:13 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/Embedded/idlexa/edito
r.pro -----

 NAME: Editor

 PURPOSE: Display an ASCII text file using widgets.

 MAJOR TOPICS: Text manipulation.

 CALLING SEQUENCE: Editor [, filename]

 INPUTS:
     Filename: A scalar string that contains the filename of the file
        to display.  The filename can include a path to that file.
        If the filename is omitted, the user will be prompted for
        a filename, via the system function, DIALOG_PICKFILE().

 KEYWORD PARAMETERS:
   FONT:   The name of the font to use.  If omitted use the default
       font.

   HEIGHT: The number of text lines that the widget should display at one
       time.  If this keyword is not specified, 24 lines is the
       default.

   WIDTH:  The number of characters wide the widget should be.  If this
       keyword is not specified, 80 characters is the default.

 PROCEDURE: Editor reads, writes and manipulates text strings ...

 MAJOR FUNCTIONS and PROCEDURES:

 COMMON BLOCKS and STRUCTURES:

 SIDE EFFECTS:
   Triggers the XMANAGER if it is not already in use.

 MODIFICATION HISTORY:  Written by:  WSO, RSI, January 1995
                        Modified by: ...
```

#XOP on-line help file: mamon.txt

MAMON

MAMON (Multiple beAM diffractiON) is an widget based graphical interface to calculate the Umweganregung peak location plot (the diffracted wavelength lambda vs. the azimutal angle angle Psi) for a given primary reflection in perfect cubic crystals.

In other words, if a crystal is set with a particular Bragg angle to match a given reflection (inputs: H,K,L) at a given wavelength (input: WaveLength), many other (secondary) reflections are excited when the crystal is rotated around the azimutal angle Psi, without changing the Bragg angle.
The plot (WaveLength,Psi) of the possible reflections is calculated and contain all possible reflection curves up to a maximum reflection (input: H Max, K Max, L Max). The intersection of these curves with an horizontal line at the wavelength of the primary reflection (input: WaveLength) gives the position of the peaks in the unweg plot. The width of each peak depends on the pendent of the curve at the intersection. For that, the Psi1 and Psi2 intersection angles with a band of width (input: DeltaWaveLength) are calculated. With this width and the intensity of the diffraction line, it is possible to compute a Gaussian that "roughly" describe the peak.

The program computes first all Miller indices hkl associated to the different crystal planes which meet the diffraction condition (multiple diffraction events) in the two-beam multiple diffraction approximation.

Translated into the reciprocal space this means that two or more knots of the reciprocal lattice come across the Ewald's sphere of radius 1/lambda (where lambda is the wavelength) at the same time when this is rotated of an angle Psi, say, about one diffraction vector P = (H,K,L).

The azimuthal angle Psi is calculated relative to an arbitrarily chosen reference direction perpendicular to the scattering vector of the primary reflection. The user can specify the energy and the angular range as well as the max hkl values considered

The theoretical frame of the program is essentially provided in:
1) B.H. Cole et al, "Simultaneous Diffraction: Indexing Umweganregungen Peaks in Simple Cases", Acta Cryst. (1962), 15, 138-144

The peak intensity is calculated with the approximated method described in:
2) K. Yvon et al., "LAZY PULVERIX, a computer program for calculating X-ray and neutron diffraction powder patterns", J. Appl. Cryst. (1977), 10, 73-74

Basically, the intensity I is calculated as I= M L P F**2, being
- M: multiplicity factor,
- P: Polarization factor,
- L: Lorentz factor (L=1/[sin_theta**2 cos_theta])
- Theta is the Bragg angle.
- F is calculated considering the scattering factor f0 calculated using using the coefficients tabulated in the file mamon.f0.

Obviously, this intensity is not correct because:
- The formula is not valid for perfect crystals, only for powders.
- The total intensity must be the sum of the primary reflection plus the intensity of the so-called operative reflections plus the contribution of the cooperative ones.
- Anomalous scattering factors are not considered.

The crystal group symmetries represented in the program are: simple cubic, body-centered cubic, face-centered cubic. In particular the selection rules for reflections peculiar of the diamond structure are also built in in the code.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

```
  File:
   MAMON input parameters: This option allows to save the current
                parameters to a file for later loading. It also allows
                to save the current parameters as defaults for being
                used when the application is initialized. In the last
                case, the file is named "application".xop (where
                "application " is the name of the current XOP
                application) and is written in the directory pointed
                by the XOP_DEFAULTS_DIR environment variable (which
                must be set). The parameter file is ASCII and can be
                read and edited with care.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                The same result is obtained pressing the "Set Parameters"
                button in the main BM window.
               Please refer to the information under the HELP
                button for a complete description of the parameters.
  Set Defaults: Sets the default parameters.

  Show: Display results
    Plot
        Spaghettis: Plots the MAMON unweganregung "spaghetti" plot results.
        Unweg: Plots the MAMON unweganregung plot, i.e., the peaks
               obtained when scanning the Psi angle. They are calculated
               from a band in the spaghetti plot centered at the
               position defined in "WaveLength" and with width equal
               to the value in DeltaWaveLength (A).
    View
        Spaghettis: Displays the MAMON output text file mamon_spaghetti.dat,
          which contains:
          h,k,l     the Miller indices of the current Umweganregung event
          theta     the cooresponding Bragg angle
          F(hkl)    the absolute value of the calculated structure factor.
                    The Debye-Waller factor is not taken into acount
          Intensity the reflection intensity
          Beta      angle between the projectons of the vectors r = (h,k,l) (whi
ch
          meets the Bragg condition at the same time as P) and
          k0 = (e0x,e0y,e0z)/lambda on the plane perpendicular to P
          [e0 is the unit vector]. Let's call these projections r_perp
                    and k0_perp, respectively
          Psi0      angle between a reference axis perpendicular to P
                    (calculated by the program) and r_perp
          Psi       rotation angle around the main diffraction vector

          calib     (not relevant for its use in this context)
                    lambda [Angstrom] as calculated from eq. 4 of ref. 1.
                    This eq. gives the relationship between primary as well as
                    operative reflection and k0 for simultaneous diffraction
                    to occur.
        Unweg: Displays the MAMON output text file mamon_unweg.dat, containing
                    the spaghetti lines that lie in the band defined by the
                    the horizontal line at WaveLength and with width DeltaWaveLe
ngth.
                    For each line that intersect, a line contains:
          Psi1:     The first intersection angle in deg.
          Psi2:     The second intersection angle in deg.
          Intensity: The curve intensity.
          H,K,L     The reflection Miller planes.

  Help:   Shows the BM help (this text).

 COPYRIGHT:
        MAMON belongs to XOP package and it is distributed within XOP.
        PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

 CREDITS:
```

Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/03-02-03

#XOP on-line help file: mamon_par.txt

Description of the input parameters for MAMON:
==========

Structure: crystal structure
a (unit cell) (A) : lattice parameter a [Angstrom] of the cubic structure investigated
Symbol: Material symbol of the crystal [e.g. Si, Ge etc]
H Maximum: max H for calculated reflection curves.
K Maximum: max K
L Maximum: max L
WaveLength (A): The wavelength (in A) for calculating the unweg pattern (the line wavelength=constant intersect the curves in the spaghetti plot).
DeltaWaveLength: the band width around WaveLength.
Psi Min (deg) : Theta_Bragg_min [deg] defining the allowed angular interval of Bragg angle of the unmweg peaks.
Psi Max (deg) : Theta_Bragg_max [deg] defining the allowed angular interval of Bragg angle of the unmweg peaks.
Psi_min and Psi_max [deg] (interval of the azimutal angle)
H
K
L (H,K,L) of the primary reflection [deg]

#XOP on-line help file: mlayer.txt

========== xmlayer ==========

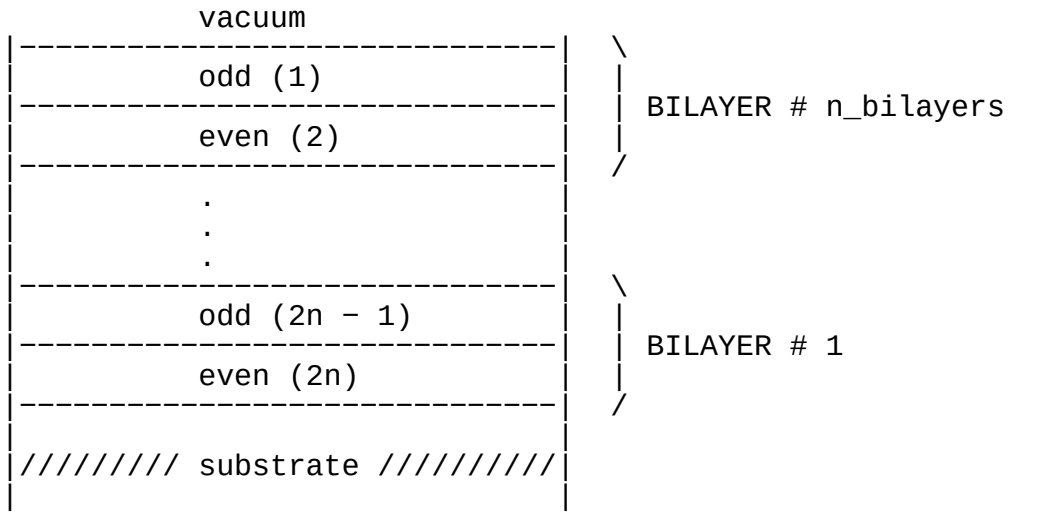
Mlayer is a widget based graphical interface to calculate multilayer reflectivities as a function of either the photon energy or incident angle.

Limitations: This code only handles elements as materials (no mixtures or compounds implemented). It does not calculate the influence of interface roughness.

***Note: The functionality of this code is quite limited. A much more performant code for multilayer calculations is IMD, available as an XOP extension.

The mlayer code has been witten by J.H. Underwood at CXRO and is part of the SHADOW package. M. Sanchez del Rio has modified it to directly call an optical library, which gives correct values of refraction indeces when the energy is scanned. M. Sanchez del Rio has also writen this graphic interface called mlayer too.

Schematic representation of the multilayer:



DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
MLayer input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main mlayer window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, mlayer starts running.
Set Defaults: Sets the default parameters.

Show: Display results
Plot Results: Plots the mlayer results.

Show/Edit material file mlayer.f12: mlayer creates the material information into a file named mlayer.f12 in the case that the "Material parameters" entry is set to "Create on the fly". However, this mlayer.f12 file can be edited by hand and reused in a next run of mlayer where the "Material parameter" entry is set to "Use existing file: mlayer.f12". This option allows the used to customize the materials, optical constants, densities, etc.
****Note that the file mlayer.f12 is overwritten when the "Material parameters" entry is set to "Create on the fly". It is also deleted when quitting the mlayer application.

Help: Shows the mlayer help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340−345, 1998.

In addition, published calculations using the mlayer aplication should also cite:

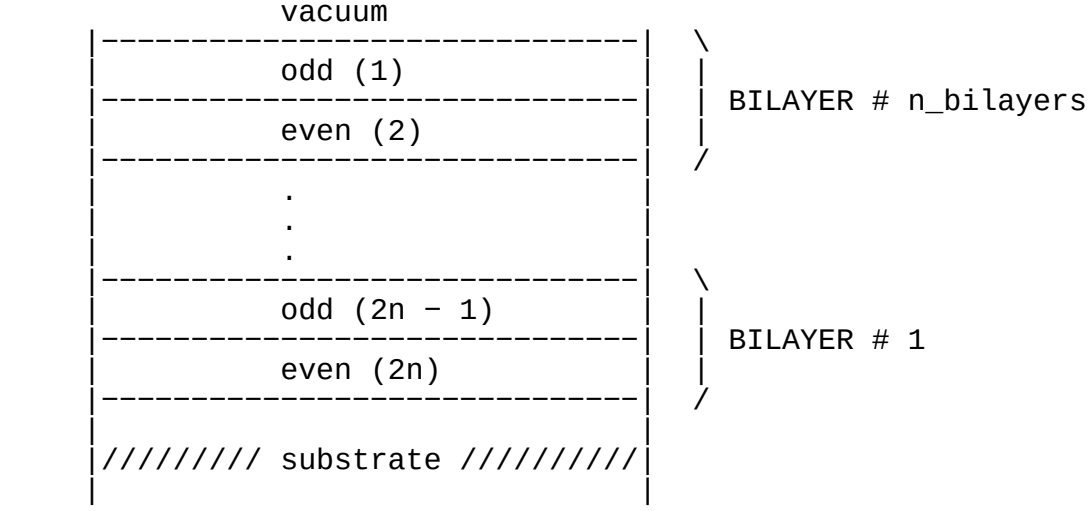
C. Welnak, G.J. Chen and F. Cerrina, "SHADOW: a synchrotron radiation X−ray Optics simulation tool",
Nucl. Instr. and Meth. in Phys. Res. A347 91994) 344
or
SHADOW WEB Page: http://www.nanotech.wisc.edu/shadow/shadow.html

LAST MODIFICATION: msr/msr/03−02−04

#XOP on-line help file: mlayer_par.txt

Description of mlayer input parameters:
==========

Schematic representation of the multilayer:



LAYER PERIODICITY: Multilayer may be periodic or aperiodic. In the first case you may define the number of layer pairs and the thickness of the two components of the pair. In the second case you must prepare a file containing two columns and N rows, one row for each pair. The first element of the column is the thickness in A of the odd element and the second column is the thickness of the even element.

SCANNING VARIABLE: Grazing angle [deg] or Photon Energy [eV]

MATERIAL PARAMETERS:
Create on the fly: the material parameters are created by mlayer and placed in a file mlayer.f12 (which overwrites previous versions).
Use existing file: mlayer.f12: Do not create the mlayer.f12 file and uses an existing one.
The mlayer.f12 file created "on the fly" can be edited by hand customize the materials, optical constants, densities, etc.

****Note that the file mlayer.f12 is overwritten when the "Material parameters" entry is set to "Create on the fly".

SUBSTRATE: Chemical symbol for the substrate.

ODD LAYER MATERIAL's chemical symbol for the odd layer

EVEN LAYER MATERIAL's chemical symbol for the even layer

PHOTON ENERGY: in eV

GRAZING ANGLE: in degrees

SCANNING VARIABLE STEP: the spep in either Photon energy or grazing angle, depending on your choice.

NUMBER OF SCANNING POINTS: obvious.

THICKNESS FOR THE ODD MATERIAL in A, when periodic Mlayers are considered.

THICKNESS FOR THE EVEN MATERIAL in A, when periodic Mlayers are considered.

NUMBER OF LAYER PAIRS when periodic Mlayers are considered.

FILE WITH LAYER THICKNESSES: file name with thicknesses as explained before, valid only when Individual layers are considered.

#XOP on-line help file: n_maxwell.txt

================================ MAXWELL ================================

Maxwell distribution is a widget based graphical interface to calculate the spectrum of neutron Maxwell source as a function of the neutron wavelength or energy.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Maxwell distribution input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialised. In the last case, the file is named "application".xop (where "application" is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
  Write Files for XOP/Optics: Saves the current neutron Maxwell source spectrum in the SRCOMPE (versus energy of neutrons in MeV) and SRCOMPW (versus wavelength of neutrons in Å) files to be used for the other XOP application from Optics menu.
  Quit: to exit from the program

Set_Parameters:
  Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main Maxwell distribution window.
  Set Defaults: Sets the default parameters.

Show: Display results
  Plot Results: Plots the Maxwell distribution results.
  View Results: Displays the Maxwell distribution outputs.

Help: Shows the Maxwell distribution help (this text).

CREDITS:
  Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: scicalc.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:14 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/Embedded/idlexa/scicalc.pro -----

NAME:
  Scicalc

PURPOSE:
  This routine emulates a scientific calculator.

CATEGORY:
  Widgets, math.

CALLING SEQUENCE:
  Scicalc

INPUTS:
  None.

KEYWORD PARAMETERS:
  GROUP: The widget ID of the widget that calls Scicalc. When this
     ID is specified, a death of the caller results in a death of
     Scicalc.

  FONT: A string containing the name of the X-Windows font to be
     used for the calculator buttons and display. If no font is
     specified, the first available 20-point font is used.
     On many systems, you can see the names of available fonts
     by entering the command "xlsfonts" from the Unix command line.

OUTPUTS:
  None.

OPTIONAL OUTPUT PARAMETERS:
  None.

COMMON BLOCKS:
  SCICALCBLOCK, WTRANSBLOCK

SIDE EFFECTS:
  Initiates the XManager if it is not already running.

RESTRICTIONS:
  Math error trapping varies depending upon system.

PROCEDURE:
  Create and register the widget, allow computations, and then exit.

MODIFICATION HISTORY:
  WIDGET CALCULATOR by Keith R Crosley, RSI, October 1991
  Created from a template written by: Steve Richards, January, 1991
      Modified by: WSO January, 1995

```
#XOP on-line help file: sync_ang.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:18 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/sync_ang.pro
-----

 NAME:
       SYNC_ANG

 PURPOSE:
       Calculates the synchrotron radiation angular distribution

 CATEGORY:
       Mathematics.

 CALLING SEQUENCE:
       Result = sync_angle(flag, angle )

 INPUTS:
        flag:   0 Flux fully integrated in photon energy
                1 Flux at a given photon energy
       amgle:  the angle array [in mrad]

 KEYWORD PARAMETERS:
        POLARIZATION: 0 Total
                      1 Parallel       (l2=1, l3=0, in Sokolov&Ternov notation)
                      2 Perpendicular  (l2=0, l3=1)

        IF FLAG=0 THE FOLLOWING KEYWORDS MUST BE ENTERED
                E_GeV= The electron energy [in GeV]
                I_A= the electron beam intensity [in A]
                HDiv_mrad= the horizontal divergence [in mrad]
                R_M= the bending magnet radius [in m]

        IF FLAG=1 THE FOLLOWING KEYWORDS MUST BE ENTERED
                All keyworsd for FLAG=0 plus:
                Energy = the energy value [in eV]
                EC_eV= The critical energy [eV]

 OUTPUTS:
       returns the array with the flux [photons/sec/0.1%bw]

 PROCEDURE:

        References:
                G K Green, "Spectra and optics of synchrotron radiation"
                        BNL 50522 report (1976)
                A A Sokolov and I M Ternov, Synchrotron Radiation,
                        Akademik-Verlag, Berlin, 1968

 MODIFICATION HISTORY:
       Written by:     M. Sanchez del Rio, srio@esrf.fr, 2002-06-03
```

```
#XOP on-line help file: sync_ene.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:18 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/sync_ene.pro
-----

 NAME:
       SYNC_ENE

 PURPOSE:
       Calculates the synchrotron radiation energy spectrum

 CATEGORY:
       Mathematics.

 CALLING SEQUENCE:
       Result = sync_ene(flag, Energy )

 INPUTS:
        flag:   0 Flux fully integrated in angle (Psi)
                1 Flux at Psi=0
                2 Flux integrated in the angular interval [Psi_Min,Psi_Max]
                3 Flux at Psi=Psi_Min

       energy:  the energy array [in eV]

 KEYWORD PARAMETERS:
        POLARIZATION: 0 Total
                      1 Parallel       (l2=1, l3=0, in Sokolov&Ternov notation)
                      2 Perpendicular  (l2=0, l3=1)

        If FLAG=0 or FLAG=1 the following keywords MUST BE ENTERED

                EC_eV= The critical energy [eV]
                E_GeV= The electron energy [in GeV]
                I_A= the electron beam intensity [in A]
                HDiv_mrad= the horizontal divergence [in mrad]

        If FLAG=2, in addition to the mentioned keywords, the following
                ones must be present:

                Psi_Min the minimum integration angle [in mrad]
                Psi_Max the maximum integration angle [in mrad]
                Psi_NPoints the number of points in psi for integration

        If FLAG=3, in addition to the mentioned keywords for FLAG=0 OR

                FLAG=1, the following kewford must be defined:
                Psi_Min the Psi angular value [in mrad]

 KEYWORD PARAMETERS (OUTPUT):

        IF FLAG=2, the following keywords can be used to obtain additional info:

                FMATRIX=A two dimensional variable containing the matrix of
                        flux as a function of angle [first index] and energy
                        [second index]
                ANGLE_MRAD= A one-dim array with the angular points [in mrad]

 OUTPUTS:
       returns the array with the flux [photons/sec/0.1%bw] for FLAG=0,2
       and the flux [photons/sec/0.1%bw/mrad] for FLAG=1,3

 PROCEDURE:

        References:
                G K Green, "Spectra and optics of synchrotron radiation"
                        BNL 50522 report (1976)
                A A Sokolov and I M Ternov, Synchrotron Radiation,
                        Akademik-Verlag, Berlin, 1968
```

EXAMPLE:
The following program was used for testing sync_ene

```
e=makearray1(10,20000.0,30000.0) ; create 10-points energy array in [20,
30] keV

;
; test of spectra at Psi=0
;
; at psi=0 (i.e., FLAG=1)
y1=sync_ene(1,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1)
; at psi_min (FLAG=3)
y2=sync_ene(3,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1,psi_min=0.0)

plot,e,y1
oplot,e,y2,Psym=2


;
; test of integrated spectra
;

; Integrating (by hand) using FLAG=3
y3 = y1*0.0D0
a = makearray1(50,-0.2,0.2)  ; it is large enough to cover the full radi
ation fan

FOR i=0,N_Elements(a)-1 DO BEGIN
  y2=sync_ene(3,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1,psi_min=a[i])
  y3 = y3 + y2
  ;plot,e,y2,title='Psi='+StrCompress(a[i])
  ;wait,0.1
ENDFOR
y3=y3*(a[1]-a[0])

; Integrating (automatically) using FLAG=2
y4 = sync_ene(2,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1,psi_min=-0.2,psi_
max=0.2,psi_npoints=50)

; Integrated (over all angles) using FLAG=0
y5 = sync_ene(0,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1)

pause
plot,e,y4
pause
oplot,e,y4,psym=2
pause
oplot,e,y5,psym=4

print,'   energy    int_by_hand     int_num    int'
FOR i=0,N_Elements(e)-1 DO BEGIN
  print,e[i],y3[i],y4[i],y5[i]
ENDFOR

end
```

The results obtained are:

energy	int_by_hand	int_num	int
20000.000	9.3255428e+12	9.3255428e+12	9.3319989e+12
21111.111	8.9528668e+12	8.9528668e+12	8.9590648e+12
22222.222	8.5885671e+12	8.5885671e+12	8.5945128e+12
23333.333	8.2334350e+12	8.2334350e+12	8.2391347e+12
24444.444	7.8880553e+12	7.8880553e+12	7.8935159e+12
25555.556	7.5528452e+12	7.5528452e+12	7.5580737e+12
26666.667	7.2280844e+12	7.2280844e+12	7.2330880e+12
27777.778	6.9139400e+12	6.9139400e+12	6.9187260e+12
28888.889	6.6104867e+12	6.6104867e+12	6.6150626e+12
30000.000	6.3177237e+12	6.3177237e+12	6.3220968e+12

```
       EXAMPLE 2
               Surface plot of flux versus angle ane energy
               e = makeArray1(20,20000,30000)
               tmp = sync_ene(2,e,ec_ev=19166.0,e_gev=6,i_a=0.1,hdiv=1,$
                       psi_min=-0.2,psi_max=0.2,psi_npoints=50,fm=fm,an=a)
               surface,fm,a,e, ztitle='Flux[phot/sec/0.1%bw/mradPsi', $
                       xtitle='Angle [mrad]',ytitle='Energy [eV]'
MODIFICATION HISTORY:
      Written by:     M. Sanchez del Rio, srio@esrf.fr, 2002-06-03
```

```
#XOP on-line help file: sync_f.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:19 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/sync_f.pro --
---
 NAME:
       SYNC_F

 PURPOSE:
       Calculates the function used for calculating the angular
        dependence of synchrotron radiation.

 CATEGORY:
       Mathematics.

 CALLING SEQUENCE:
       Result = sync_hi(rAngle [,rEnergy] )

 INPUTS:
       rAngle:  the reduced angle, i.e., angle[rads]*Gamma. It can be a
                scalar or a vector.
 OPTIONAL INPUTS:
       rEnergy:  a value for the reduced photon energy, i.e.,
                energy/critical_energy. It can be an scalar or a verctor.
                If this input is present, the calculation is done for this
                energy. Otherwise, the calculation results is the integration
                over all photon energies.

 KEYWORD PARAMETERS:
        POLARIZATION: 0 Total
                      1 Parallel       (l2=1, l3=0, in Sokolov&Ternov notation)
                      2 Perpendicular  (l2=0, l3=1)

        L2: The polarization value of L2
        L3: The polarization value of L3
                Note: If using L2 and L3, both L2 and L3 must be defined.
                      In this case, the Pol keyword is ignored.

        GAUSS: When this keyword is set, the "Gaussian" approximaxion
                instead of the full calculation is used.
                Only valid for integrated flux aver all photon energies.
 OUTPUTS:
       returns the value  of the sync_f function
                It is a scalar if both inputs are scalar. If one input
                is an array, the result is an array of the same dimension.
                If both inputs are arrays, the resulting array has dimension
                NxM, N=Dim(rAngle) and M=Dim(rEnergy)

 PROCEDURE:
       The number of emitted photons versus vertical angle Psi is
        proportional to sync_f, which value is given by the formulas
        in the references.

        For angular distribution integrated over full photon energies (rEnergy
        optional input not present) we use the Formula 9, pag 4 in Green.
        For its gaussian approximation (in this case the polarization keyword
        has no effect) we use for 87 in pag 32 in Green.

        For angular distribution at a given photon energy (rEnergy
        optional input not present) we use the Formula 11, pag 6 in Green.


        References:
                G K Green, "Spectra and optics of synchrotron radiation"
                        BNL 50522 report (1976)
                A A Sokolov and I M Ternov, Synchrotron Radiation,
                        Akademik-Verlag, Berlin, 1968

 OUTPUTS:
```

```
      returns the value  of the sync_hi function

PROCEDURE:
      Uses IDL's BeselK() function

MODIFICATION HISTORY:
      Written by:     M. Sanchez del Rio, srio@esrf.fr, 2002-05-23
       2002-07-12 srio@esrf.fr adds circulat polarization term for
                wavelength integrated spectrum (S&T formula 5.25)
```

```
#XOP on-line help file: sync_g1.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:19 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/sync_g1.pro -
----
 NAME:
       SYNC_G1

 PURPOSE:
       Calculates the functions used for calculating synchrotron
        radiation energy spectrum integrated over the full vertical
        angle.

 CATEGORY:
       Mathematics.

 CALLING SEQUENCE:
       Result = sync_g1(x)

 INPUTS:
       x:      the argument of the function. It is converted to double
                precision for calculations.

 KEYWORD PARAMETERS:
        POLARIZATION: 0 Total
                      1 Parallel       (l2=1, l3=0, in Sokolov&Ternov notation)
                      2 Perpendicular  (l2=0, l3=1)
 OUTPUTS:
       returns the value  of the sync_g1 function

 PROCEDURE:
       The number of emitted photons versus energy is:
        N(E) = 2.4605e13 I[A] Ee[Gev] Theta[mrad] Sync_G1(E/Ec]
           Where:
                I is the storage ring intensity in A
                Ee is the energy of the electrons in the storage ring
                E is the photon energy
                Ec is the critical energy
                The value Sync_G1 returned by this function is:
                Sync_G1(x) (total polarization):
                    x* Integrate[BeselK[x,5/3],{x,y,Infinity}]
                Sync_G1(x,Pol=1) (parallel polarization):
                    (1/2)* [x* Integrate[BeselK[x,5/3],{x,y,Infinity}] +
                    x*BeselK(x,2/3)]
                Sync_G1(x,Pol=2) (perpendicular polarization):
                    (1/2)* [x* Integrate[BeselK[x,5/3],{x,y,Infinity}] -
                    x*BeselK(x,2/3)]

        For calculating the Integrate[BeselK[x,5/3],{x,y,Infinity}]
                        function, the function fintk53 is used.

        Reference: A A Sokolov and I M Ternov, Synchrotron Radiation,
                         Akademik-Verlag, Berlin, 1968, Formula 5.19,
                         pag 32.

 MODIFICATION HISTORY:
       Written by:     M. Sanchez del Rio, srio@esrf.fr, 2002-05-24
```

```
#XOP on-line help file: sync_hi.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:19 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/sync_hi.pro -
----
 NAME:
       SYNC_HI

 PURPOSE:
       Calculates the function Hi(x) used for Synchrotron radiation
        Hi(x) = x^i * BeselK(x/2,2/3) (for total polarization)


 CATEGORY:
       Mathematics.

 CALLING SEQUENCE:
       Result = sync_hi(x [,i] )

 INPUTS:
       x:      the argument of the function. All calculations are done in doble
               precision.
        i:      the exponent. If this optional argument is not entered, it
                is set to 2.

 KEYWORD PARAMETERS:
        POLARIZATION: 0 Total
                      1 Parallel       (l2=1, l3=0, in Sokolov&Ternov notation)
                      2 Perpendicular  (l2=0, l3=1)

 OUTPUTS:
       returns the value  of the sync_hi function

 PROCEDURE:
       Uses the relation ship Hi(x) =  x^i * sync_f(0,x)

 MODIFICATION HISTORY:
       Written by:     M. Sanchez del Rio, srio@esrf.fr, 2002-05-23
```

#XOP on-line help file: tasmip_par.txt

Description of the input parameters for XTUBE_W:
==========

VOLTAGE: anode voltage in kiloVolts (in the 30-140 interval)
VOLTAGE RIPPLE: RMS value in %
AL FILTER: Al filtration: layer thickness in mm

```
#XOP on-line help file: tc.txt

Last modification date of this file: Mon Nov 17 00:09:32 CST 1997
Roger J. Dejus (dejus@aps.anl.gov)
C+
C PROGRAM DESCRIPTION:
C  Program to calculate on-axis brilliance tuning curves for an ideal undulator
C  insertion device (regular planar device or a helical device). The program
C  uses the Bessel function approximation which is valid for an ideal device,
C  e.g., no magnetic field errors. The effect of the particle beam emittance and
C  the beam energy spread is taken into account.
C
C AUTHORS:
C  Roger J. Dejus
C  The Advanced Photon Source
C  Experimental Facilities Division
C  Argonne National Laboratory
C
C CREATION DATE:
C  22-APR-1996
C
C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the undulator device, and the brilliance calculation.
C Machine Parameters:
C  ENERGY               Storage ring energy              (GeV)
C  CUR                  Storage ring current             (mA)
C  SIGE                 Energy spread (sigma(E)/E)
C  SIGX                 RMS beam size (horizontal)       (mm)
C  SIGY                 RMS beam size (vertical)         (mm)
C  SIGX1                RMS beam divergence (horizontal) (mrad)
C  SIGY1                RMS beam divergence (vertical)   (mrad)
C Undulator Parameters:
C  PERIOD               Undulator period length          (cm)
C  N                    Number of periods
C Scan Parameters:
C  EMIN                 Lower energy limit for FIRST harmonic (eV)
C  EMAX                 Upper energy limit for FIRST harmonic (eV)
C  NE                   Number of energy points
C  IHMIN                Minimum harmonic of interest
C  IHMAX                Maximum harmonic of interest
C  IHSTEP               Step size for the harmonics
C Brilliance Parameters:
C  IHEL                 Type of device; ihel=0: regular planar, ihel=1: helical
C  METHOD               Method
C                       METHOD={0,1}Non-zero emittance;
C                                   infinite-N +convolution (Dejus' approach)
C                       METHOD=2    Non-zero emittance;
C                                   infinite-N +convolution (Walker's approach)
C                       METHOD=3    Non-zero emittance; finite-N (Walker's)
C
C  IK                   Print K-values & powers; ik=0: quiet, ik=1: print
C  NEKS                 Number of energy points for peak search: Default 100, or
C                       use 0 for default.
C COMMON BLOCKS:
C  None.
C
C DESIGN ISSUES:
C  The down shift in energy due to the beam emittance is most noticable for
C  small values of K, and therefore, for each harmonic, the energy shift is
C  calculated for K = Kmin. The shifted peak is then used to define the energy
C  interval over which the on-axis brilliance is calculated. The peak of this
C  function is stored and subsequently saved in a file vs. energy (eV). The
C  user enters the scanning range in energy (eV) for the first harmonic, even in
C  the case when higher harmonics are chosen (using IHMIN > 1). The beam energy
C  spread is included by using a straightforward convolution at the fixed energy
C  of the peak. Beam energy spreads typically in the range 1% to 0.01% can be
C  used. It is valid to set the beam energy spread to zero. The number of energy
C  points for peak search NEKS is used at each K-value and would typically be
C  set to the default value unless the down shift in energy is being sought with
```

```
C  high accuracy. For high accuracy typically use NEKS = 1000.
C
C COPYRIGHT:
C  Unless part of the XOP software package, this routine must only be used
C  at The Advanced Photon Source and must not be tranferred or used at any
C  other location without the written consent of the author.
C
C FILES USED:
C Input files
C  tc.dat
C Output files
C  tc.plt
C
C KEYWORDS:
C  Undulator Tuning Curve, Undulator On-Axis Brilliance.
C
C LINK/LIBRARY ISSUES:
C  Calls routine USB that calls routines BRIGHTE and HUNT.
C  BRIGHTE calculates the brightness and HUNT searches an array of real
C  numbers (from Numerical Recipes).
C
C PORTABILITY ISSUES:
C  Runs on DEC 3000/400 AXP alpha (Unix 4.0b) and SUN (Solaris: SunOS Release
C  5.5.1)
C
C TIMING:
C  Generally, the execution is fast. For example, the first three odd
C  harmonics (1, 3, 5) for Undulatar A at the APS over the full tuning range is
C  calculated in about 10 s using the default parameters for the infinite-N
C  method with convolution and zero beam energy spread. The finite-N method is
C  about 10 times slower. Introduction of the beam energy spread increases the
C  execution time by typically 40%. The timing above is given for the default
C  value of NEKS (=100) and the number of points/harmonic ne = 20.
C
C VERSION:
C  1.9
C
C MODIFICATION HISTORY:
C        Date     | Name  | Description
C ----------------+-------+-----------------------------------------------------
C 10-MAY-1996     | RJD   | Tuning variable is K.
C ----------------+-------+-----------------------------------------------------
C 21-MAY-1996     | RJD   | Changed tuning variable to E1 and added descriptive
C                 |       | text describing the input/output. First official
C                 |       | release, v1.2.
C ----------------+-------+-----------------------------------------------------
C 13-MAR-1997     | RJD   | Added beam energy spread using a straightforward
C                 |       | convolution at the fixed energy of the peak.
C                 |       | Modified calculation of the variable nek. Added the
C                 |       | variable ik which controls printing of K-values.
C                 |       | Current version is v1.3.
C ----------------+-------+-----------------------------------------------------
C 18-MAR-1997     | RJD   | Modified upper limit of peak search from 1.0 to
C                 |       | fc2 = 1.002. Added parameter SPECLIM which defines
C                 |       | the minimum Brilliance to retain in the calculation.
C                 |       | Current version is v1.4.
C ----------------+-------+-----------------------------------------------------
C 21-MAR-1997     | RJD   | Modified lower limit of peak search from fc =
C                 |       | 0.990d0*ep/eiz to fc = 0.985d0*ep/eiz so that the
C                 |       | the peak of the higher odd harmonics will be found
C                 |       | (or is more likely to be found) when the beam energy
C                 |       | spread is taken into account.
C                 |       | Current version is v1.5.
C ----------------+-------+-----------------------------------------------------
C 15-JUL-1997     | RJD   | Added information about total emitted power and
C                 |       | on-axis power density to the printout when the print
C                 |       | variable ik is set to 1. Current version is v1.6.
C ----------------+-------+-----------------------------------------------------
C 29-SEP-1997     | RJD   | Added printout of zero emittance energy (first
C                 |       | column in output file). Current version is v1.7.
```

```
C ----------------+-------+----------------------------------------------------
C 06-OCT-1997     | RJD   | The parameter NEKS which determines the number of
C                 |       | energy points for the peak search at each K-value
C                 |       | was added to the input file. Default = 100 (or enter
C                 |       | 0). Min and max is 100 and 10000, respectively.
C ----------------+-------+----------------------------------------------------
C 14-NOV-1997     | RJD   | The variable neks declared as integer*4.
C                 |       | Current version is v1.9.
C ----------------+-------+----------------------------------------------------
C-
```

```
#XOP on-line help file: tc_par.txt

C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the undulator device, and the brilliance calculation.
C Machine Parameters:
C  ENERGY               Storage ring energy              (GeV)
C  CUR                  Storage ring current             (mA)
C  SIGE                 Energy spread (sigma(E)/E)
C  SIGX                 RMS beam size (horizontal)       (mm)
C  SIGY                 RMS beam size (vertical)         (mm)
C  SIGX1                RMS beam divergence (horizontal) (mrad)
C  SIGY1                RMS beam divergence (vertical)   (mrad)
C Undulator Parameters:
C  PERIOD               Undulator period length          (cm)
C  N                    Number of periods
C Scan Parameters:
C  EMIN                 Lower energy limit for FIRST harmonic (eV)
C  EMAX                 Upper energy limit for FIRST harmonic (eV)
C  NE                   Number of energy points
C  IHMIN                Minimum harmonic of interest
C  IHMAX                Maximum harmonic of interest
C  IHSTEP               Step size for the harmonics
C Brilliance Parameters:
C  IHEL                 Type of device; ihel=0: regular planar, ihel=1: helical
C  METHOD               Method
C                       METHOD={0,1}Non-zero emittance;
C                                   infinite-N +convolution (Dejus' approach)
C                       METHOD=2    Non-zero emittance;
C                                   infinite-N +convolution (Walker's approach)
C                       METHOD=3    Non-zero emittance; finite-N (Walker's)
C
C  IK                   Print K-values & powers; ik=0: quiet, ik=1: print
C  NEKS                 Number of energy points for peak search: Default 100, or
C                       use 0 for default.
```

#XOP on-line help file: urgent.txt

```
**************************************************************************
**************************************************************************

!!    UU      UU  RRRRRR      GGGGGGG  EEEEEEEE  NNN      NN  TTTTTTTTTT    !!
!!    UU      UU  RR   RR   GGGGGGGGG  EE        NNNN     NN  TTTTTTTTTT    !!
!!    UU      UU  RR   RR  GGG         EE        NN NN    NN      TT        !!
!!    UU      UU  RR  RR   GG          EEEEEEE   NN  NN   NN      TT        !!
!!    UU      UU  RRRRR    GG    GGGG  EEEEEEE   NN   NN  NN      TT        !!
      UU      UU  RR  RR   GGG     GG  EE        NN    NN NN      TT
!!    UUU    UUU  RR   RR   GGGGGGGGG  EE        NN     NNNN      TT        !!
!!     UUUUUUUU   RR    RR    GGGGGGG  EEEEEEEE  NN      NNN      TT        !!

**************************************************************************
**************************************************************************
```

A program for calculating Undulator Radiation properties.

Authors : R.P.Walker and B.Diviacco, Sincrotrone Trieste

Reference : R.P.Walker and B.Diviacco,
Proc. 4th Int. Conf. Synchrotron Radiation Instrumentation, Chester, July 1991,
to be published in Rev. Sci. Instrum. Jan. 1992,
Sincrotrone Trieste report ST/M-91/12

Modification record :
06/11/89 - Version 1
first distributed version
19/03/90 - Version 1.1
changes in output format to include power information
new MODE=6 for radiation power calculations
addition of beam current parameter (CUR)
elimination of an error in MODE=1 ICALC=1
15/05/90 - Version 2
includes polarization parameters and eliptical
trajectories (KX, KY parameters)
04/09/91 - Version 3.0
includes crossed undulator
new definition of l4
changes to MODE=6 method of calculation and parameters
various other small changes

```
**************************************************************************
```

The following are complete up-to-date instructions for running URGENT.
Please use the latest version available.

1. INTRODUCTION

URGENT is designed for the accurate and efficient calculation of the basic properties (angular, spectral, polarization, power density) of the radiation generated in ideal plane, helical or elliptical undulators, and also the crossed-undulators scheme [Nikitin,Kim].

It can take into account :
- non-zero electron beam emittance (size and divergence)
- finite number of undulator periods (N)
- multiple harmonics contributing at a given photon energy

but also has options for :
- zero emittance
- infinite N
- single harmonic

The main approximations are :
- ideal electron trajectory (i.e. no tapering or field errors)
- far-field.

It is written in standard FORTRAN 77, calls no library routines, and needs no graphics package and so should be easily transportable.

URGENT uses the Bessel function method to calculate the basic radiation angular flux density function in an efficient manner. An appropriate choice is made of routine depending on whether the magnet is plane or helical, in order to minimize cpu time.

2. DATA INPUT

The data is read on unit 5 (FOR005) in free−format (READ(5,*)). There are 6 lines, containing the following parameters :

1) ITYPE, PERIOD, KX, KY, PHASE, N
2) EMIN, EMAX, NE
3) ENERGY, CUR, SIGX, SIGY, SIGX1, SIGY1
4) D, XPC, YPC, XPS, YPS, NXP, NYP
5) MODE, ICALC, IHARM
6) NPHI, NSIG, NALPHA, DALPHA, NOMEGA, DOMEGA

A value must be entered for each parameter, even if not relevant for the calculation that is to be performed. Parameters ITYPE, N, NE, NXP, NYP, MODE, ICALC, IHARM, NPHI, NSIG, NALPHA, NOMEGA are integers.

The parameters have the following meaning :

Line 1 : Undulator
ITYPE − either ITYPE=1 : plane/helical/elliptical magnet
or ITYPE=2 : crossed undulator
PERIOD − magnet period (m)
KX, KY − magnet deflection parameters coresponding to a horizontal and vertical field direction respectively
PHASE − phase difference between the two undulators in the crossed undulator scheme (degrees)
N − number of magnet periods

Line 2 : Photon Energy
EMIN − minimum photon energy (eV) (>0)
EMAX − maximum photon energy (eV)
NE − number of photon energy intervals (<5000)

Line 3 : Electron Beam
ENERGY − electron beam energy (GeV)
CUR − electron beam current (A)
SIGX, SIGY − rms horizontal and vertical electron beam sizes (mm)
SIGX1, SIGY1 − rms horizontal and vertical electron beam divergences (mrad)

Line 4 : Observation point and range of acceptance
D − distance from centre of undulator to the observation point (m)
XPC, YPC − horizontal and vertical position of the observation point or centre of the range of acceptance (mm or mrad)
XPS, YPS − TOTAL horizontal and vertical acceptance (mm or mrad)
NXP, NYP − number of intervals into which the acceptance is divided in the horizontal and vertical directions (<50)

Line 5 : Calculation Method
MODE − type of calculation, having the following possible values :
MODE=1 angular/spatial flux density distribution at photon energy EMIN
In this case EMAX, NE are irrelevant.
MODE=2 spectrum of angular/spatial flux density at position XPC, YPC
In this case XPS, YPS, NXP and NYP are irrelevant.
MODE=3 spectrum of on−axis brightness.
In this case D, XPC, YPC, XPS, YPS, NXP and NYP are irrelevant.
MODE=4 spectrum of flux integrated over the defined range of acceptance.
MODE=5 spectrum of flux integrated over all angles
In this case D, XPC, YPC, XPS, YPS, NXP and NYP are irrelevant.
MODE=6 angular/spatial distribution of power density in a given harmonic or range of harmonics; central power density and integrated power over the range of acceptance, listed for each harmonic
In this case EMIN, EMAX, NE are irrelevant
Note : to increase the options available MODE=−6 can also

be used (see below under IHARM).

ICALC − calculation method, having the following possible values :
   For MODE=1,2,3,4 : ICALC=1 non−zero emittance, finite N
                       ICALC=2 non−zero emittance, infinite N
                       ICALC=3 zero emittance, finite N
   For MODE=5 :   ICALC=1 finite N
                       ICALC=2 infinite N
   For MODE=6 :   ICALC=1 non−zero emittance
                       ICALC=2 zero emittance

IHARM − number of harmonics to be included, having the following values :
   For MODE=1,2,3,4,5 with ICALC=1,2 :
            IHARM=−1 include all harmonics contributing at a
            given point and given photon energy
            IHARM=0 use only the lowest order contributing harmonic
            IHARM=i use only the i'th harmonic
   For MODE=1,2,3,4 with ICALC=3 : IHARM is not relevant
   For MODE=6 :
         IHARM=i angular/spatial distribution of power density for harmonic i
         IHARM=−i include all harmonics from 1 to i
            MODE=−6 :
            angular/spatial distribution of power density for each harmonic
          + angular/spatial distribution of power density for sum of harmonics
          + central power density and integrated power for each i
            MODE=6 :
            angular/spatial distribution of power density for sum of harmonics
          + central power density and integrated power for each i
         IHARM=0 include harmonics up to some limit determined by the program
            MODE=−6 or MODE=6 as above

LINE 6 : Calculation Parameters
− All of the following parameters can be set to zero in which
case they default to the values given in brackets [].

NPHI −   no. of steps in phi between 0 and pi/2.0 [20]. NPHI < 100.
         used in (MODE=1,2,3,4,5 ICALC=1,2)
NSIG −   no. of standard deviations of electron beam dimensions (size and
         divergence) to be included [4].
         used in (MODE=1,2,3,4 ICALC=1,2) and (MODE=6 ICALC=1)
NALPHA − no. of steps in angle alpha (gamma*theta) [15]. NALPHA < 100.
         used in (MODE=1 ICALC=1).
DALPHA − range of angles in alpha**2 to be used, in units of the angular
         equivalent of 1/N [2.0].
         used in (MODE=1 ICALC=1) and ICALC=3.
NOMEGA − no. of steps in photon energy for the natural lineshape [16].
         NOMEGA < 5000.
         used in (MODE=2,3,4,5 ICALC=1)
DOMEGA − range of photon energies to be included in the natural lineshape
         in units (energy of fundamental/N) [2.0] i.e. the default value
         covers the range +/− 2/N of the natural lineshape.
         used in (MODE=2,3,4,5 ICALC=1)

NOTES :

i/ For (MODE=2,3,4,5 ICALC=1 ITYPE=1) the finite N spectrum is obtained by
convoluting the infinite N spectrum with the natural lineshape.
To make this easy the point spacing in photon energy must be the same
for the two curves. This can be achieved as follows :
− set NE=0, in which case the spacing is set by the values of NOMEGA and
  DOMEGA and NE is set accordingly.
− set NE to the approximate number of points desired in the energy range
  EMIN,EMAX. A new value of NE is then calculated which gives the closest
  match with the spacing of the natural lineshape.
In either case EMAX will also be adjusted so that the convolution
can be carried out correctly over the defined energy region.
In order to get an accurate convolution the program insists that
the rule (NOMEGA/DOMEGA) >= 4 is respected.

ii/ In cases with non−zero emittance (MODE=1,2,3,4,ICALC=1,2 and MODE=6, ICALC=1) both SIGX and SIGY may be zero, but both SIGX1 and SIGY1 must be non−zero.

iii/ If D is set to zero, this indicates that angular flux and power density is to be calculated rather than spatial flux and power density in MODEs 1,2,4 and 6. In this case SIGX and SIGY are ignored, and the acceptance (XPC, YPC, XPS, YPS) is entered in mrad rather than mm units.

iv/ If the acceptance is centred on the axis (XPC=YPC=0.0) then only one quarter of the acceptance needs to be calculated because of symmetry. In this case the range from (0,0) to (XPS/2.0,YPS/2.0) will be divided into NXP, NYP intervals. The printed values of integrated flux and power, including Stokes parameters will however be correct for the total acceptance.

v/ Theta (alpha/gamma) is the angle between the undulator axis and the direction of observation. Phi is the angle between the projection of the angle of observation in the x−y plane and the x−axis.

vi/ MODE=6 : In addition to power density the program now also prints total flux density (photons/s/mrad**2 or mm**2), and as well as integrated power the total flux (photons/s). The central value means at the centre of the defined acceptance in the case of a 2D acceptance (NXP>0, NYP>0). In other cases it refers to the first point. It is permitted to enter NXP=0 or NYP=0 to obtain values of the power density for example as a function of vertical or horizontal position (angle) respectively.

vii/ For the crossed undulator (ITYPE=2) the following special rules apply :
− KX is set to 0.0; both undulators are assummed to have deflection parameter KY
− each undulator is assumed to have N periods
− only MODE = 1, 2 or 4 can be used
− NPHI <= 25
− The calculation method is different to that for standard magnets (ITYPE=1); finite N is taken into account directly and no convolution with the natural lineshape is necessary. ICALC=1 or ICALC=2 can be entered equally; NOMEGA and DOMEGA are irrelevant. DALPHA is needed in all cases, NALPHA for ICALC=1,2.

3. DATA OUTPUT

Data are output on unit 6 (FOR006). In all cases the main data start on line 33.

The input parameters are firstly printed. Parameters on lines 1,2,4,6 that are not relevant for the type of calculation required are set to zero. The on−axis photon energy and wavelength, and the total power and peak power density (zero emittance) are also given. The power density is only given for the plane and helical (KX=KY) case.

The units used throughout are as follows :

Photon energy	[eV]
Wavelength	[Angstrom]
Spatial flux density=Irradiance	[photons/s/mm**2/0.1%bandwidth]
Angular flux density	[photons/s/mrad**2/0.1%bandwidth]
Brightness	[photons/s/mm**2/mrad**2/0.1%bandwidth]
Flux	[photons/s/0.1%bandwidth]
Spectral power density	[Watts/mm**2 or mrad**2/eV bandwidth]
Power density	[Watts/mm**2 or mrad**2]
Spectral power	[Watts/eV bandwidth]
Power	[Watts]

4. POLARIZATION

Angular/spatial flux densities and integrated flux are given in terms of polarization parameters l1, l2, l3, l4 where :

l1 = s1/s0 l2 = s2/s0 l3 = s3/s0

and l4 = 1 − sqrt((l1**2)+(l2**2)+(l3**2))

s0, s1, s2 and s3 are the Stokes parameters, integrated over the beam emittance, range of acceptance etc. :

s0 = total intensity
s1 = difference in intensity between radiation polarized linearly in the horizontal direction and in the vertical direction
s2 = difference in intensity between radiation polarized linearly in the directions at +45 degrees and −45 degrees with respect to the horizontal and vertical directions
s3 = difference in intensity between radiation polarized circularly in the right−handed and left−handed sense

Thus, the fraction of radiation that is polarized is

sqrt((l1**2)+(l2**2)+(l3**2))

and l4 represents the fraction of radiation that is unpolarized.
l1, l2 and l3 vary between −1 and +1; l4 varies between 0 and 1.
Note the change in definition of l4 from URGENT version 2. It now is in agreement with the definition of Born and Wolf, Principles of Optics p.555.

With the assumption that the undulator fields are parallel to the x and y axes, and that electron beam distributions that are symmetrical with respect to the x and y axes −
In general : l2 = 0 on−axis, or with an acceptance that is symmetric with respect to the x and y axes
In a plane undulator (KX=0, KY#0) : l3 = 0 always

5. COMMENTS AND SUGGESTIONS

In a program of this sort it is impossible to guarantee that sensible results will be obtained in all circumstances. Thus, the user should (as with any reasonably complicated computer program) judge himself whether the results are sensible by the usual techniques of changing the input parameters (e.g. number of energy intervals, number of points in the acceptance etc.) in order to check that the results remain reasonably consistent, or change in the expected way (changing for example the emittance parameters, or choosing options for infinite N etc.)

In most cases the default values for parameters in line 6 are appropriate, i.e. enter 0 0 0 0 0 0.

The default values should give accurate values of the flux to a level of the order 0.1% of the main peak. If accuracy is wanted to lower values, it may be necessary to increase NSIG (e.g. 6).

For MODE=1,2,3,4,5 if in doubt use IHARM=−1; the data output will include information on which harmonics were actually used in the calculation.

For MODE=2,3,4,5 there is little difference in the calculation time for spectra with ICALC=1 or 2, however ICALC=2 allows the photon energy interval to be set independently of any natural lineshape criterion, which can be useful for either a preliminary calculation or in some particular cases [e.g. at high photon energies compared to the first harmonic where the infinite N approximation is a good approximation to the finite N result].

For cases with small emittance and small photon energy ICALC=3 can be a reasonable approximation (MODE=1,2,3,4).

For cases with large emittance and large photon energy ICALC=2 can be a reasonable approximation (MODE=1,2,3,4).

For MODE=6, when the electron beam emittance (divergence) is small compared to 1/gamma, ICALC=2 is a good approximation. When the emittance and pinhole are sufficiently small that different harmonics in the spectrum do not overlap, the power density and integrated power in the individual harmonics can conveniently be calculated directly (IHARM=0), rather than by spectral calculations for each separate harmonic.

Some problems can occur in computing spectra in the case with small emittance and small photon energy i.e. the "diffraction limited" case. Here it is necessary to make sure that the infinite N spectrum first calculated by the program is sensible − i.e. has sufficient points in it (determined by the photon energy interval used) and in the case of integrating over a pinhole is suitably "smooth" (determined by the

spacing of points in the pinhole). A reasonable criterion for the latter is that the spacing XPS/NXP should be as follows :

XPS/NXP < 2.0 * SQRT((SIGX*SIGX)+(D*D*SIGX1*SIGX1))

and the same in the vertical plane.

6. USING THE PROGRAM

The FORTRAN source program comes in a single part : URGENT.FOR which should be compiled and linked to form an executable program. No external routines are called. Although the program has been developed on a VAX, it compiles under FOR/STANDARD and has also been compiled on a PC.

Most calculations can be performed in an interactive mode in a few seconds to a few minutes cpu time. A simple VAX COM file to run the program URGENT.EXE reading the data from INP.DAT and outputing to OUT.DAT is as follows :

```
$ ASSIGN INP.DAT FOR005
$ ASSIGN OUT.DAT FOR006
$ RUN URGENT
$ DEASS FOR005
$ DEASS FOR006
$ EXIT
```

A sample input file is as follows :

```
1 0.056 0.0 3.39 0.0 81
295. 303. 0
2.0 0.4 0.228 0.044 0.033 0.017
20.0   0. 0. 2. 2. 10 10
4 1 3
0 0 0 0 0 0
```

In this example the flux is integrated over a 2 mm x 2 mm pinhole 20 m from the source, for a 5.6 cm period undulator in ELETTRA at 2 GeV 400mA, near the third harmonic. The photon energy range is defined, but not the interval − which is determined by the program for compatibility with the natural lineshape. For this run the calculation time on a VAXSTATION 3100/MOD.30 is 21 s for 27 photon energy points.

7. PROGRAM DISTRIBUTION and FURTHER INFORMATION

The program may be freely copied to anyone else who would like it. However, it is in the best interest of anyone who uses the program to let me know so that they can receive further updates of the program.

Anyone who has difficulty in using the program and requires advice should feel free to contact me. Comments on the operation of the program and suggestions for new developments would also be welcome.

Communication is preferred by e−mail :

Bitnet − R.WALKER@ELETTRA.TRIESTE.IT
DecNet − SYNCTS::WALKER or 40082::WALKER

alternatively :

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fax. 39−40−226338

R.P.Walker,

September 4th, 1991

#XOP on-line help file: urgent_par.txt

2. DATA INPUT

The data is read on unit 5 (FOR005) in free-format (READ(5,*)).
There are 6 lines, containing the following parameters :

1) ITYPE, PERIOD, KX, KY, PHASE, N
2) EMIN, EMAX, NE
3) ENERGY, CUR, SIGX, SIGY, SIGX1, SIGY1
4) D, XPC, YPC, XPS, YPS, NXP, NYP
5) MODE, ICALC, IHARM
6) NPHI, NSIG, NALPHA, DALPHA, NOMEGA, DOMEGA

A value must be entered for each parameter, even if not relevant for the calculation that is to be performed. Parameters ITYPE, N, NE, NXP, NYP, MODE, ICALC, IHARM, NPHI, NSIG, NALPHA, NOMEGA are integers.

The parameters have the following meaning :

Line 1 : Undulator
ITYPE - either ITYPE=1 : plane/helical/elliptical magnet
or ITYPE=2 : crossed undulator
PERIOD - magnet period (m)
KX, KY - magnet deflection parameters coresponding to a horizontal and vertical field direction respectively
PHASE - phase difference between the two undulators in the crossed undulator scheme (degrees)
N - number of magnet periods

Line 2 : Photon Energy
EMIN - minimum photon energy (eV) (>0)
EMAX - maximum photon energy (eV)
NE - number of photon energy intervals (<5000)

Line 3 : Electron Beam
ENERGY - electron beam energy (GeV)
CUR - electron beam current (A)
SIGX, SIGY - rms horizontal and vertical electron beam sizes (mm)
SIGX1, SIGY1 - rms horizontal and vertical electron beam divergences (mrad)

Line 4 : Observation point and range of acceptance
D - distance from centre of undulator to the observation point (m)
XPC, YPC - horizontal and vertical position of the observation point or centre of the range of acceptance (mm or mrad)
XPS, YPS - TOTAL horizontal and vertical acceptance (mm or mrad)
NXP, NYP - number of intervals into which the acceptance is divided in the horizontal and vertical directions (<50)

Line 5 : Calculation Method
MODE - type of calculation, having the following possible values :
MODE=1 angular/spatial flux density distribution at photon energy EMIN
In this case EMAX, NE are irrelevant.
MODE=2 spectrum of angular/spatial flux density at position XPC, YPC
In this case XPS, YPS, NXP and NYP are irrelevant.
MODE=3 spectrum of on-axis brightness.
In this case D, XPC, YPC, XPS, YPS, NXP and NYP are irrelevant.
MODE=4 spectrum of flux integrated over the defined range of acceptance.
MODE=5 spectrum of flux integrated over all angles
In this case D, XPC, YPC, XPS, YPS, NXP and NYP are irrelevant.
MODE=6 angular/spatial distribution of power density in a given harmonic or range of harmonics; central power density and integrated power over the range of acceptance, listed for each harmonic
In this case EMIN, EMAX, NE are irrelevant
Note : to increase the options available MODE=-6 can also be used (see below under IHARM).

ICALC - calculation method, having the following possible values :
For MODE=1,2,3,4 : ICALC=1 non-zero emittance, finite N
ICALC=2 non-zero emittance, infinite N

```
                        ICALC=3 zero emittance, finite N
   For MODE=5 :         ICALC=1 finite N
                        ICALC=2 infinite N
   For MODE=6 :         ICALC=1 non-zero emittance
                        ICALC=2 zero emittance

IHARM - number of harmonics to be included, having the following values :
   For MODE=1,2,3,4,5 with ICALC=1,2 :
             IHARM=-1 include all harmonics contributing at a
             given point and given photon energy
             IHARM=0 use only the lowest order contributing harmonic
             IHARM=i use only the i'th harmonic
   For MODE=1,2,3,4 with ICALC=3 : IHARM is not relevant
   For MODE=6 :
         IHARM=i  angular/spatial distribution of power density for harmonic i
         IHARM=-i include all harmonics from 1 to i
            MODE=-6 :
            angular/spatial distribution of power density for each harmonic
          + angular/spatial distribution of power density for sum of harmonics
          + central power density and integrated power for each i
            MODE=6 :
            angular/spatial distribution of power density for sum of harmonics
          + central power density and integrated power for each i
         IHARM=0  include harmonics up to some limit determined by the program
            MODE=-6 or MODE=6 as above

LINE 6 : Calculation Parameters
- All of the following parameters can be set to zero in which
case they default to the values given in brackets [].

NPHI -   no. of steps in phi between 0 and pi/2.0 [20]. NPHI < 100.
         used in (MODE=1,2,3,4,5 ICALC=1,2)
NSIG -   no. of standard deviations of electron beam dimensions (size and
         divergence) to be included [4].
         used in (MODE=1,2,3,4 ICALC=1,2) and (MODE=6 ICALC=1)
NALPHA - no. of steps in angle alpha (gamma*theta) [15]. NALPHA < 100.
         used in (MODE=1 ICALC=1).
DALPHA - range of angles in alpha**2 to be used, in units of the angular
         equivalent of 1/N [2.0].
         used in (MODE=1 ICALC=1) and ICALC=3.
NOMEGA - no. of steps in photon energy for the natural lineshape [16].
         NOMEGA < 5000.
         used in (MODE=2,3,4,5 ICALC=1)
DOMEGA - range of photon energies to be included in the natural lineshape
         in units (energy of fundamental/N) [2.0] i.e. the default value
         covers the range +/- 2/N of the natural lineshape.
         used in (MODE=2,3,4,5 ICALC=1)


NOTES :

i/ For (MODE=2,3,4,5 ICALC=1 ITYPE=1) the finite N spectrum is obtained by
convoluting the infinite N spectrum with the natural lineshape.
To make this easy the point spacing in photon energy must be the same
for the two curves. This can be achieved as follows :
- set NE=0, in which case the spacing is set by the values of NOMEGA and
  DOMEGA and NE is set accordingly.
- set NE to the approximate number of points desired in the energy range
  EMIN,EMAX. A new value of NE is then calculated which gives the closest
  match with the spacing of the natural lineshape.
In either case  EMAX will also be adjusted so that the convolution
can be carried out correctly over the defined energy region.
In order to get an accurate convolution the program insists that
the rule (NOMEGA/DOMEGA) >= 4 is respected.

ii/ In cases with non-zero emittance (MODE=1,2,3,4,ICALC=1,2 and MODE=6,
ICALC=1) both SIGX and SIGY may be zero, but both SIGX1 and SIGY1 must
be non-zero.

iii/ If D is set to zero, this indicates that angular flux and power density
```

is to be calculated rather than spatial flux and power density in MODEs 1,2,4 and 6. In this case SIGX and SIGY are ignored, and the acceptance (XPC, YPC, XPS, YPS) is entered in mrad rather than mm units.

iv/ If the acceptance is centred on the axis (XPC=YPC=0.0) then only one quarter of the acceptance needs to be calculated because of symmetry. In this case the range from (0,0) to (XPS/2.0,YPS/2.0) will be divided into NXP, NYP intervals. The printed values of integrated flux and power, including Stokes parameters will however be correct for the total acceptance.

v/ Theta (alpha/gamma) is the angle between the undulator axis and the direction of observation. Phi is the angle between the projection of the angle of observation in the x−y plane and the x−axis.

vi/ MODE=6 : In addition to power density the program now also prints total flux density (photons/s/mrad**2 or mm**2), and as well as integrated power the total flux (photons/s). The central value means at the centre of the defined acceptance in the case of a 2D acceptance (NXP>0, NYP>0). In other cases it refers to the first point. It is permitted to enter NXP=0 or NYP=0 to obtain values of the power density for example as a function of vertical or horizontal position (angle) respectively.

vii/ For the crossed undulator (ITYPE=2) the following special rules apply :
− KX is set to 0.0; both undulators are assummed to have deflection parameter KY
− each undulator is assumed to have N periods
− only MODE = 1, 2 or 4 can be used
− NPHI <= 25
− The calculation method is different to that for standard magnets (ITYPE=1); finite N is taken into account directly and no convolution with the natural lineshape is necessary. ICALC=1 or ICALC=2 can be entered equally; NOMEGA and DOMEGA are irrelevant. DALPHA is needed in all cases, NALPHA for ICALC=1,2.

```
#XOP on-line help file: us.txt

Last modification date of this file: Mon Nov 17 00:19:40 CST 1997
Roger J. Dejus (dejus@aps.anl.gov)
C+
C PROGRAM DESCRIPTION:
C  Program to calculate undulator spectra within the Bessel function
C  approximation for an ideal planar undulator or an ideal elliptical
C  undulator (including polarization in both cases).
C  The program may be executed from the xop interface.
C
C AUTHORS:
C  Roger J. Dejus
C  The Advanced Photon Source
C  Experimental Facilities Division
C  Argonne National Laboratory
C
C CREATION DATE:
C  25-MAR-1991
C
C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the undulator device, and the quantity to be calculated. Note: When modifying
C  parameters under the Xus interface, double click the field and make sure to
C  press the RETURN key so that the new parameter is accepted.
C Machine Parameters:
C  Storage ring energy                  (GeV)
C  Storage ring current                 (mA)
C  RMS beam size (horizontal)           (mm)
C  RMS beam size (vertical)             (mm)
C  RMS beam divergence (horizontal)     (mrad)
C  RMS beam divergence (vertical)       (mrad)
C Undulator Parameters:
C  Period length                       (cm)
C  Number of periods
C  Deflection parameter (hor.  field) Kx (= 0.0 for a regular planar device)
C  Deflection parameter (vert. field) Ky
C Scan Parameters:
C  Minimum energy                      (eV)
C  Maximum energy                      (eV)
C  Number of energy points
C Pinhole Parameters:
C  Distance from the source            (m)
C    (d=0.0 => angular units)
C  X-coordinate for center of pinhole   (mm) or (mrad)
C  Y-coordinate for center of pinhole   (mm) or (mrad)
C  X-size of pinhole (full width)       (mm) or (mrad)
C  Y-size of pinhole (full width)       (mm) or (mrad)
C    (for angular units (d=0.0) values are entered in mrad)
C    (X is for horizontal direction)
C    (Y is for the vertical direction)
C  Number of subdivisions of pinhole in X (max 50)
C  Number of subdivisions of pinhole in Y (max 50)
C    (for plotting 3d results with Xus, the X-size, Y-size, and the number of
C     of subdivisions in the two directions should be equal)
C
C Mode:
C  Depending on the mode selected, some of the pinhole parameters may be
C  set to different values by the program; see the output file us.plt.
C  MODE    1    Angular/spatial flux density distribution
C  MODE    2    Angular/spatial flux density spectrum
C  MODE    3    On-axis brilliance spectrum
C  MODE    4    Flux spectrum through a pinhole
C  MODE    5    Flux spectrum integrated over all angles
C  MODE    6    Power density and integrated power
C
C  Angular/spatial flux density distribution
C    - Flux distribution at the energy chosen as minimum energy.
C  Angular/spatial flux density spectrum
C    - Spectrum at any given point in space as selected by the X and Y
```

```
C      coordinate for the center of the pinhole. X is horizontal and Y is
C      vertical.
C  On-axis brilliance spectrum
C  Flux spectrum through a pinhole
C    - Spectrum through a pinhole centered at X-center and Y-center with
C      size X-size and Y-size.  The energy range is from the minimum to the
C      maximum energy.
C  Flux spectrum integrated over all angles.
C    -  The pinhole parameters have no significance here.
C  Power density and integrated power
C    -  Integrated over all energies, thus the energy parameters have no
C       significance here.
C
C Method:
C  METHOD  1    Non-zero emittance; finite-N
C  METHOD  2    Non-zero emittance; infinite-N
C  METHOD  3    Zero emittance;     finite-N
C  METHOD  4    Non-zero emittance; infinite-N + convolution (Dejus' approach)
C  METHOD 14    Non-zero emittance; infinite-N + convolution (Walker's approach)
C
C  Non-zero emittance; finite-N
C    - Use only for "Angular/spatial flux density distribution" and for
C      "Power density and integrated power".
C  Non-zero emittance; infinite-N
C    - For test purposes; do not use (will be removed from menu).
C  Zero emittance; finite-N
C    - Use for zero emittance calculations.
C  Non-zero emittance; infinite-N/convolution
C    - Generally, use for cases where emittance should be included.
C
C Harmonic Number:
C  IHARM   0    All harmonics
C  IHARM  -1    Lowest order harmonic (except MODE=6, include to -IHARM)
C  IHARM   I    I'th harmonic
C
C  All harmonics
C    - Selects all contributing harmonics (generally used).
C  Lowest order harmonic
C    - Selects the lowest order contributing harmonic.
C  Harmonic #
C    - Selects the harmonic number displayed.
C  Edit harmonic number
C    - Modifies the displayed harmonic number.
C
C Intrinsic Parameters:
C  Several parameters used in the calculations.  Usually not modified by the
C  user.  Please see me (RJD) for further information.
C
C Polarization:
C  The normalized Stokes parameters are calculated including the
C  unpolarized component.
C
C DESIGN ISSUES:
C  Program is based on the Bessel function approximation and is valid in the
C  far-field for an ideal sinusoidal magnetic field profile.
C
C COPYRIGHT:
C  Unless part of the XOP software package, this routine must only be used
C  at The Advanced Photon Source and must not be tranferred or used at any
C  other location without the written consent of the author.
C
C FILES USED:
C  Input file - us.dat  File in the user's current directory containing the
C                       input parameters.
C  Output file - us.plt File in the user's current directory containing the
C                       results of the calculation.  The header contains
C                       all input parameters and the calculated zero emittance
C                       on-axis first harmonic energy (e1), corresponding
C                       wavelength (l1), total power (ptot), and the on-axis
C                       power density (pd).
```

```
C KEYWORDS:
C  Undulator Spectrum, Bessel Function Approximation
C
C LINK/LIBRARY ISSUES:
C  Calls routines BRIGHTE and HUNT.  BRIGHTE calculates the brilliance and HUNT
C  searches an array of real numbers (from Numerical Recipes).
C
C PORTABILITY ISSUES:
C  Runs on DEC 3000/400 AXP alpha (Unix v. 3.2c), SUNs (SUN-OS 4.1.3),
C  HP 9000/735-series (HP-UX 9.03).
C
C TIMING:
C  Execution times vary considerably depending on computer and the
C  quantity being calculated.  The zero emittance calculations are fast
C  (few seconds), whereas the non-zero emittance calculations may range from
C  seconds (on-axis brilliance) to an hour (flux spectrum through a pinhole).
C
C VERSION:
C  1.9
C
C MODIFICATION HISTORY:
C
C        Date     | Name  | Description
C ----------------+-------+-----------------------------------------------------
C 06-JUL-1994     | RJD   | Modified value for E1MIN for angle-integrated
C                 |       | spectrum (MODE=5) to be non-zero; gamma*theta
C                 |       | corresponds to sqrt(200) (somewhat arbitrarily
C                 |       | chosen)
C ----------------+-------+-----------------------------------------------------
C 04-OCT-1994     | RJD   | Modified program to include polarization properties.
C                 |       | The four Stokes parameters are now calculated.
C                 |       | Program is for an ideal planar undulator or an ideal
C                 |       | elliptical undulator. Many other changes. The value
C                 |       | of the parameter IHARM has a different meaning.
C                 |       | IHARM=0 now gives 'all harmonics' and IHARM= <0
C                 |       | gives the lowest order harmonic except for the power
C                 |       | option. For the power option, a negative IHARM means
C                 |       | include all harmonics up to and including -IHARM.
C                 |       | This version is 1.6.
C ----------------+-------+-----------------------------------------------------
C 21-JUN-1995     | RJD   | Modified print-out of "Contributing harmonics" in
C                 |       | subroutine PRINT_OUT. Routine incorrectly calculated

C                 |       | IMIN and IMAX for METHOD 4 (Dejus' method) for
C                 |       | "Spectral distributions". The spectra and integrated
C                 |       | quantities were calculated correctly and are
C                 |       | unaffected by this modification.
C                 |       | The current version is 1.7.
C ----------------+-------+-----------------------------------------------------
C 04-JAN-1996     | RJD   | Modified the number of decimal places for the sigx1
C                 |       | and sigy1 variables to four in the printout. Added
C                 |       | one more digit for the emax variable to avoid
C                 |       | overflow on rare occasions. Formats 260 and 256 were
C                 |       | changed accordingly.
C                 |       | The current version is 1.8.
C ----------------+-------+-----------------------------------------------------
C 11-NOV-1997     | RJD   | Changed notation: Brightness -> Brilliance.
C                 |       | The current version is 1.9.
C ----------------+-------+-----------------------------------------------------
C [change_entry]
C-
```

```
#XOP on-line help file: us_par.txt

C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the undulator device, and the quantity to be calculated. Note: When modifying
C  parameters under the Xus interface, double click the field and make sure to
C  press the RETURN key so that the new parameter is accepted.
C Machine Parameters:
C  Storage ring energy                  (GeV)
C  Storage ring current                 (mA)
C  RMS beam size (horizontal)           (mm)
C  RMS beam size (vertical)             (mm)
C  RMS beam divergence (horizontal)     (mrad)
C  RMS beam divergence (vertical)       (mrad)
C Undulator Parameters:
C  Period length                        (cm)
C  Number of periods
C  Deflection parameter (hor.  field) Kx (= 0.0 for a regular planar device)
C  Deflection parameter (vert. field) Ky
C Scan Parameters:
C  Minimum energy                       (eV)
C  Maximum energy                       (eV)
C  Number of energy points
C Pinhole Parameters:
C  Distance from the source             (m)
C    (d=0.0 => angular units)
C  X-coordinate for center of pinhole   (mm) or (mrad)
C  Y-coordinate for center of pinhole   (mm) or (mrad)
C  X-size of pinhole (full width)       (mm) or (mrad)
C  Y-size of pinhole (full width)       (mm) or (mrad)
C    (for angular units (d=0.0) values are entered in mrad)
C    (X is for horizontal direction)
C    (Y is for the vertical direction)
C  Number of subdivisions of pinhole in X (max 50)
C  Number of subdivisions of pinhole in Y (max 50)
C    (for plotting 3d results with Xus, the X-size, Y-size, and the number of
C     of subdivisions in the two directions should be equal)
```

#XOP on-line help file: ws.txt

========== Xws ==========

Xws is an widget based graphical interface to calculate spectral properties of a wiggler insertion device.

The main window contains four buttons:

QUIT: Exits from the program

DATA: Defines the parameters for the calculation

SHOW: Plots, Prints or Views the results

HELP: Shows the Xws help text or the WS help text

Author: Roger J. Dejus (dejus@anlaps.aps.anl.gov), APS, May, 1994.
Modification history:
96/01/19 MSR changes labels Xtransmit -> XOP/Optics
97/01/23 MSR changes for Windows95, cosmetics (xhelp, widget_message...)
97/02/05 MSR adds help button in parameters window.
97/10/02 MSR uses sdep(), xop_wd and other cosmetics.
00/07/17 MSR introduces ws 1.5 in the interface.

```
C+
C PROGRAM DESCRIPTION:
C  Program to calculate wiggler and bending magnet spectra using the
C  Bessel function approximation. The program may be executed from the xop
C  interface.
C
C AUTHORS:
C  Roger J. Dejus
C  The Advanced Photon Source
C  Experimental Facilities Division
C  Argonne National Laboratory
C
C CREATION DATE:
C  17-FEB-1994
C
C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the wiggler device, and the quantity to be calculated.
C Machine Parameters:
C  Storage ring energy                  (GeV)
C  Storage ring current                 (mA)
C Wiggler Parameters:
C  Period length                        (cm)
C  Number of periods
C Note: For a bending magnet source: set N=0.5, and make Ky large and adjust
C       the period length accordingly. For example, put Ky=9.34 and calculate
C       the period length from, Period (cm) = 10.0/B0(T), where B0 is the known
C       strength of the magnetic field (in Tesla) for the bending magnet.  The
C       calculated power density (pd) is correct, but the total power (ptot)
C       is irrelevant. Typically make the extend of the pinhole small in the
C       horizontal direction (theta << Ky/gamma) as the intensity should
C       not depend on the horizontal offset. Check value of B0 (and critcal
C       energy EC0) in the plot file.
C  Deflection parameter (hor.  field) Kx (= 0.0 only; for elliptical wiggler
C  not yet implemented)
C  Deflection parameter (vert. field) Ky
C Scan Parameters:
C  Minimum energy                       (eV)
C  Maximum energy                       (eV)
C  Number of energy points
C Pinhole Parameters:
C  Distance from the source             (m)
```

```
C    (d=0.0 => angular units)
C  X-coordinate for center of pinhole   (mm) or (mrad)
C  Y-coordinate for center of pinhole   (mm) or (mrad)
C  X-size of pinhole (full width)       (mm) or (mrad)
C  Y-size of pinhole (full width)       (mm) or (mrad)
C    (for angular units (d=0.0) values are entered in mrad)
C    (X is for horizontal direction)
C    (Y is for the vertical direction)
C  Number of subdivisions of pinhole in X (max 50)
C  Number of subdivisions of pinhole in Y (max 50)
C
C Mode:
C  Depending on the mode selected, some of the pinhole parameters may be
C  set to different values by the program; see the output file ws.plt.
C  MODE    1    Angular/spatial flux density distribution
C  MODE    2    Angular/spatial flux density spectrum
C  MODE    3    On-axis brilliance spectrum (not yet implemented)
C  MODE    4    Flux spectrum through a pinhole
C  MODE    5    Flux spectrum integrated over all angles
C  MODE    6    Power density and integrated power
C
C  Angular/spatial flux density distribution
C    - Flux distribution at the energy chosen as minimum energy.
C  Angular/spatial flux density spectrum
C    - Spectrum at any given point in space as selected by the X and Y
C      coordinate for the center of the pinhole. X is horizontal and Y is
C      vertical.
C  On-axis brilliance spectrum (not yet implemented)
C  Flux spectrum through a pinhole
C    - Spectrum through a pinhole centered at X-center and Y-center with
C      size X-size and Y-size.  The energy range is from the minimum to the
C      maximum energy.
C  Flux spectrum integrated over all angles (wiggler only).
C    -  The pinhole parameters have no significance here.
C  Power density and integrated power
C    -  Integrated over all energies, thus the energy parameters have no
C       significance here.
C
C Polarization:
C  The normalized Stokes parameters are calculated including the
C  unpolarized component.
C
C DESIGN ISSUES:
C  Program calculates the spectra from the Modified Bessel functions.  See K.J.
C  Kim, in "Physics of Particle Accelerators", vol. 1, AIP Conference Proc. 184
C  Ed. R.G. Lerner, New York (1989), p. 583, Eq. (3.12).
C  The algorithm is based on a series expansion for small arguments Z
C  (Abramowitz & Stegun Eq. 9.6.2 and 9.6.10) and an asymptotic expansion for
C  large arguments (Eq. 9.7.2).
C  Reference: Handbook of Mathematical Functions, Eds. Milton Abramowitz and
C  Irene A. Stegun, Ninth Printing, Dover Publications, New York (1970).
C  NOTE: THE POLARIZATION PARAMETERS ARE PROVIDED ALTHOUGH NOT THOROUGHLY
C  TESTED - USE WITH CAUTION.
C
C COPYRIGHT:
C  Unless part of the XOP software package, this routine must only be used
C  at The Advanced Photon Source and must not be tranferred or used at any
C  other location without the written consent of the author.
C
C FILES USED:
C  Input file - ws.dat  File in the user's current directory containing the
C                       input parameters.
C  Output file - ws.plt File in the user's current directory containing the
C                       results of the calculation.  The header contains
C                       all input parameters and the calculated on-axis first
C                       harmonic energy (e1), corresponding wavelength (l1),
C                       total power (ptot), and the on-axis power density (pd).
C                       See note above when using N=0.5 for bending magnet.
C KEYWORDS:
C  Wiggler Spectrum, Modified Bessel Function of Second kind.
```

```
C
C LINK/LIBRARY ISSUES:
C  The gamma function is needed.  Currently uses no library routines. The values
C  for gamma(2/3) and gamma(1/3) are stored as constants. May be substituted by
C  calls to the NAG library routine S14AAF.
C
C PORTABILITY ISSUES:
C  Runs on DEC 3000/400 AXP alpha (Tru64Unix v5.0), SUN (Solaris: SunOS
C  Release v5.6), and Windows 95/98/NT (Pentium and higher).
C
C TIMING:
C  Execution time is typically very fast but depends on the quantity being
C  calculated. Typically seconds to at the most minutes.
C
C VERSION:
C  1.5
C
C MODIFICATION HISTORY:
C
C        Date     | Name  | Description
C ----------------+-------+-----------------------------------------------------
C 17-JUL-2000     | RJD   | Adopted from v1.4 which was never released to the
C                 |       | public. Turned off circular polarization for the
C                 |       | wiggler (which is only valid for EMW).
C                 |       | Current version is v1.5.
C ----------------+-------+-----------------------------------------------------
C [change_entry]
C-
```

```
#XOP on-line help file: ws_par.txt

C INPUT PARAMETERS:
C  The input parameters are divided into sections related to the storage ring,
C  the wiggler device, and the quantity to be calculated.
C Machine Parameters:
C  Storage ring energy                    (GeV)
C  Storage ring current                   (mA)
C Wiggler Parameters:
C  Period length                         (cm)
C  Number of periods
C Note: For a bending magnet source: set N=0.5, and make Ky large and adjust
C       the period length accordingly. For example, put Ky=9.34 and calculate
C       the period length from, Period (cm) = 10.0/B0(T), where B0 is the known
C       strength of the magnetic field (in Tesla) for the bending magnet.  The
C       calculated power density (pd) is correct, but the total power (ptot)
C       is irrelevant. Typically make the extend of the pinhole small in the
C       horizontal direction (theta << Ky/gamma) as the intensity should
C       not depend on the horizontal offset. Check value of B0 (and critcal
C       energy EC0) in the plot file.
C  Deflection parameter (hor.  field) Kx (= 0.0 only; for elliptical wiggler
C  not yet implemented)
C  Deflection parameter (vert. field) Ky
C Scan Parameters:
C  Minimum energy                       (eV)
C  Maximum energy                       (eV)
C  Number of energy points
C Pinhole Parameters:
C  Distance from the source             (m)
C    (d=0.0 => angular units)
C  X-coordinate for center of pinhole   (mm) or (mrad)
C  Y-coordinate for center of pinhole   (mm) or (mrad)
C  X-size of pinhole (full width)       (mm) or (mrad)
C  Y-size of pinhole (full width)       (mm) or (mrad)
C    (for angular units (d=0.0) values are entered in mrad)
C    (X is for horizontal direction)
C    (Y is for the vertical direction)
C  Number of subdivisions of pinhole in X (max 50)
C  Number of subdivisions of pinhole in Y (max 50)
C
C Mode:
C  Depending on the mode selected, some of the pinhole parameters may be
C  set to different values by the program; see the output file ws.plt.
C  MODE    1    Angular/spatial flux density distribution
C  MODE    2    Angular/spatial flux density spectrum
C  MODE    3    On-axis brilliance spectrum (not yet implemented)
C  MODE    4    Flux spectrum through a pinhole
C  MODE    5    Flux spectrum integrated over all angles
C  MODE    6    Power density and integrated power
C
C  Angular/spatial flux density distribution
C    - Flux distribution at the energy chosen as minimum energy.
C  Angular/spatial flux density spectrum
C    - Spectrum at any given point in space as selected by the X and Y
C      coordinate for the center of the pinhole. X is horizontal and Y is
C      vertical.
C  On-axis brilliance spectrum (not yet implemented)
C  Flux spectrum through a pinhole
C    - Spectrum through a pinhole centered at X-center and Y-center with
C      size X-size and Y-size.  The energy range is from the minimum to the
C      maximum energy.
C  Flux spectrum integrated over all angles (wiggler only).
C    -  The pinhole parameters have no significance here.
C  Power density and integrated power
C    -  Integrated over all energies, thus the energy parameters have no
C       significance here.
C
C Polarization:
C  The normalized Stokes parameters are calculated including the
C  unpolarized component.
```

C

#XOP on-line help file: xbfield.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:18 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xbfield.pro -
----

============================ Xbfield   ==================================

   Xbfield is an widget based graphical interface to calculate
   field of an tappered undulator insertion devices.

************************ IMPORTANT NOTICE **********************************
   This utility (coming with the YAUP distribution), in the tapered case,
   generates a B field assumed be an amplitude-modulated sinusoid, e.g.
   Btot(z) = B(z)*sin(2*pi/period*z) and a linearly modulated gap is
   assumed. DG is the degree of gap taper:
   gap=gzmin*(1.0+z*dg/ulen)
   r=gap/per
   ampl=0.95*3.44*exp(-r*(5.08-1.54*r)) (for Nb-Fe-B magnets) or
   ampl=0.95*3.33*exp(-r*(5.47-1.80*r)) (for Sm-Co magnets). This
   approximation comes from "6 GeV Synchrotron X-ray Source, Conceptual
   Design Report Supplement A", LS-52, Argonne National Laboratory,
   (March 1986), and you can also find it in the ESRF Foundation Phase
   Report (The red book), pag CIV-314

   If these parameters does not fit with the user's requirements, then
   the user should either customize it or create another bfield
   program which writes the output magnetic field in the format
   accepted by yaup.
****

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    XBField input parameters: This option allows to save the current
                parameters to a file for later loading. It also allows
                to save the current parameters as defaults for being
                used when the application is initialized. In the last
                case, the file is named "application".xop (where
                "application " is the name of the current XOP
                application) and is written in the directory pointed
                by the XOP_DEFAULTS_DIR environment variable (which
                must be set). The parameter file is ASCII and can be
                read and edited with care.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                The same result is obtained pressing the "Set Parameters"
                button in the main XBField window.
               Please refer to the information under the HELP
                button for a complete description of the parameters. After
                pressing the ACCEPT button, BFIELD starts running.
  Set Defaults: Sets the default parameters.

  Show: Display results
    Plot Results: Plots the BFIELD results.
    Show Numerical Results: Displays the BFIELD result file.

  Help: Shows the BFIELD help and the XBFIELD help (this text).

 COPYRIGHT:
        xyaup and xbfield belong to XOP package and are distributed within XOP.
        PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

 CREDITS:
        Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations using the YAUP package should also cite:

B. I. Boyanov, G. Bunker, J. M. Lee, and T. I. Morrison
"Numerical Modeling of Tapered Undulators"
Nucl. Instr. Meth. A339, 596-603, 1994

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xbfield_par.txt

Description of the input parameters for xbfield

PERIOD: magnet period in cm.

N: number of periods

NPTS: Number of points per period (for internal use in calculations)

Undulator magnet: Magnet composition (Nd-Fe-B of Sm-Co)

Undulator type: Plane (convensional) or tapered undulator

K: Deflection parameter K

For tapared undulators define:
  GAP: initial gap in cm.
  GAPTAP: Gap taper in %

FILE: The output file name.

It uses a linearly modulated gap model of the form (see BFIELD.F):

B=0.95*3.44*exp(-r*(5.08-1.54*r))

where B is the magnetic field
      r = lgap/period
      lgap is the "local" gap, i.e., lgap=GAP*(1.0+z*(GAPTAP/100)/PERIOD)
      z is the spatial position along the undulator axis

#XOP on-line help file: xcom.txt

XCOM: Photon Cross Sections on a Personal Computer

M. J. Berger and J. H. Hubbell
Center for Radiation Research
National Bureau of Standards
Gaithersburg, MD 20899

A computer program and data base are presented which can be used to calculate, with a personal computer, photon cross sections for scattering, photoelectric absorption and pair production, as well as total attenuation coefficients, in any element, compound or mixture, at energies from 1 keV to 100 GeV.

1. Introduction

Data on the scattering and absorption of photons (x-rays, gamma rays, bremsstrahlung) are required for many scientific, engineering and medical applications. The number of materials for which photon cross sections are needed is large and ever increasing. Available tables [1-11] usually include cross sections for many (but not all) elements. Some tables [1,2,6,11] also contain data for a limited number of compounds and mixtures. In practice it is not possible to meet all cross-section requirements adequately by means of printed tables. Moreover, the cross sections are often needed at photon energies other than those included in the tables.

Photon cross sections for compounds can of course be obtained rather accurately (except at energies close to absorption edges) as weighted sums of the cross sections for the atomic constituents. However, the required numerical work is tedious, and the task is further complicated by the fact that photoabsorption cross sections and total attenuation coefficients are discontinuous at absorption edges. The presence of these discontinuities makes it desirable that cross section tables for compounds include photon energies immediately above and below all the absorption edges for all the atomic constituents, and this requires much additional interpolation.

A convenient alternative approach is to generate the cross sections and attenuation coefficients for compounds and mixtures as needed, using a personal computer. This paper describes a computer program called XCOM which carries out this task quickly on IBM-compatible personal computers, for any element, compound or mixture, at energies between 1 keV and 100 GeV. The program makes use of a database of cross sections for the elements that is stored in compressed form on a single floppy disk.

The XCOM program can generate cross sections on a standard energy grid (spaced approximately logarithmically), or on a grid selected by the user, or for a mix of both grids. Cross sections at energies immediately above and below all absorption edges are automatically included. XCOM provides two forms of output: (a) tables which correspond closely in format to existing tables in the literature; (b) user-selected arrays which are convenient for further computer calculations.

The program provides total cross sections and attenuation coefficients as well as partial cross sections for the following processes: incoherent scattering, coherent scattering, photoelectric absorption, and pair production in the field of the atomic nucleus and in the field of the atomic electrons. For compounds, the quantities tabulated are partial and total mass interaction coefficients, which are equal to the product of the corresponding cross sections times the number of target molecules per unit mass of the material. The reciprocals of these interaction coefficients are the mean free paths between scatterings, between photo-electric absorption events, or between pair production events. The sum of the interaction

coefficients for the individual processes is equal to the total attenuation coefficient. Total attenuation coefficients without the contribution from coherent scattering are also given, because they are often used in gamma-ray transport calculations.

The interaction coefficients and total attenuation coefficients for compounds or mixtures are obtained as sums of the corresponding quantities for the atomic constituents. The weighting factors, that is, the fractions by weight of the constituents, are calculated by XCOM from the chemical formula entered by the user. For mixtures, however, the user must supply the fractions by weight of the various components.

Some limitations should be noted. The cross sections for elements in the XCOM database pertain to isolated neutral atoms, and do not take into account molecular and solid-state effects which modify the cross sections, especially in the vicinity of absorption edges. Relatively small cross sections, such as those for Delbruck scattering, two-photon Compton scattering or photo-meson production, are not included. Also omitted is the nuclear photoeffect which, in the giant-dipole resonance region from 5 to 30 MeV, can contribute a few percent to the total attenuation coefficient. Finally, XCOM does not calculate energy absorption coefficients that represent the conversion of photon energy to kinetic energy of secondary Compton-, photo-, and pair-electrons.

2. Database for Elements

A comprehensive database for all elements over a wide range of energies was constructed through the combination of incoherent and coherent scattering cross sections from Refs. [12] and [13], photoelectric absorption from Scofield [14], and pair production cross sections from Ref. [8]. For scattering and pair production, the same cross sections are used as in other recent tabulations in Refs. [6, 8, and 11], whereas for photoelectric absorption there is a small difference (omission of a renormalization correction) which is discussed below.

The incoherent (Compton) scattering cross sections in Ref. [12] were obtained from a combination of the Klein-Nishina formula and nonrelativistic Hartree-Fock incoherent scattering functions. Radiative and double Compton-scattering corrections were also included. The coherent (Rayleigh) scattering cross sections in Ref. [13] were calculated from a combination of the Thompson formula and relativistic Hartree-Fock atomic form factors. The photoelectric cross sections were obtained by Scofield [14] by a phase-shift calculation for a central potential and a Hartree-Slater atomic model. Scofield's results extend only up to 1.5 MeV. At higher energies, where the photoelectric cross section is quite small, a semi-empirical formula from Ref. [2] connects Scofield's values at 1.5 MeV to the asymptotic high-energy limit calculated by Pratt [15]. Cross sections for pair production given in Ref. [8] are based on complicated combinations of formulas from Bethe-Heitler theory with various other theoretical models to take into account screening, Coulomb, and radiative corrections. Different combinations were used in the near-threshold, intermediate and high-energy regions to obtain the best possible agreement with experimental cross sections.

For elements with atomic numbers from 2 to 54, Scofield [14] presented correction factors for individual atomic subshells, with which the photo-effect cross sections can be renormalized so that they correspond approximately to a relativistic Hartree-Fock model rather than the Hartree-Slater model used in the original calculation. This renormalization is most significant for the outer atomic shells; the total cross section is lowered by no more than 10 percent at energies above 1 keV. Scofield did not actually apply the renormalization to the cross sections given in his tables. The renormalization was used, however, in the tabulations in Refs. [6, 8, and 11]. Recent reviews [16,17] indicate that, on the whole, agreement with experiment is better when the renormalization is not done. We have therefore omitted the renormalization in the database for the XCOM program.

3. Interpolation and Combination

For the purpose of interpolation with respect to photon energy, the

coherent and incoherent scattering cross sections and the total attenuation coefficients are approximated by log–log cubic–spline fits as functions of energy. For the pair–production cross sections, the fitted quantity is the logarithm of the quantity ((1–E'/E)**3)*SPAIR(E), where E is the photon energy , E' the threshold energy for pair production, and SPAIR(E) is the cross section. The fitting is done separately for pair production in the field of the atomic nucleus (E' = 1.022 MeV) and in the field of the atomic electrons (E' = 2.044 MeV).

The combined photoelectric absorption cross section for all shells is similarly interpolated with use of log–log cubic–spline fits, but only at energies above the K–shell absorption edge. Below this energy, interpolation is applied to the logarithm of the photoelectric absorption cross section for each separate shell, fitted as a linear function of the logarithm of the photon energy. The separate fitting for each shell is necessary to avoid the error that would be incurred by interpolating across absorption edges. Linear log–log fitting is equivalent to assuming that the photoelectric cross section is proportional to a power of the photon energy, and was found to provide more satisfactory fits than a log–log cubic–spline fit near the absorption edges.

The interaction coefficients and total attenuation coefficients for compounds are obtained as weighted sums over the corresponding coefficients for elements. XCOM automatically calculates the weight factors, i.e., the fractions by weights of the atomic constituents, from the chemical formula for the compound entered by the user. For mixtures, the user must enter the fractions by weight of the components.

4. Overview of the XCOM Program

The hardware requirements for running the XCOM program are moderate. It is sufficient to have an IBM–compatible personal computer with a memory of at least 256K bytes, and with at least one 5.25–inch floppy–disk drive. It is assumed that the computer is operated with the PC–DOS or an MS–DOS operating system, version 2.0 or later. A mathematical co–processor (Intel 8087 or 80287 chip) is not required, but is highly desirable, because it speeds up to execution of XCOM by a factor of twenty or better.

The XCOM program is distributed on two 5.25–inch floppy disks. One of these is the Database Disk, and contains 100 data files designated as MDAT.001, MDAT.002, ..., MDAT.100. These files, generated by a Fortran program and written in binary format, contain the cross–section database for the elements with atomic numbers Z = 1 to 100. The other disk is the Program Disk, and contains an executable file called XCOM.EXE.

The Program Disk also contains a copy of this report, in file XCOM.DOC, and the Fortran source code for XCOM. The source code is not needed to run XCOM. It is included to make it possible for the user to make modify the program, and to adapt the program to for use with a different operating system or computer.

The main program, XCOM, uses the following subroutines:

SPEC — Allows the user to specify the composition of the material, the energy list, desired output etc.

FORM — Translates the chemical symbols for elements or chemical formulas for compounds into the composition of the material specified in terms of atomic numbers, atomic weights, and fractions by weight of the atomic constituents.

MERGE — Creates a merged energy list arranged according to magnitude. This list combines a standard energy grid (approximately logarithmic) with the set of absorption–edge energies for all the atomic constituents for a given compound or mixture, and with the set of additional energies which the user wishes to add.

REV Utility routine for reversing the order of certain arrays.

SCOF Routine for generating coefficients for cubic−spline fits.

BSPOL Interpolation routine (based on binary search) making use of cubic−spline interpolation coefficients from SCOF.FOR.

BLIN Linear interpolation routine, based on binary search.

Also included on the Program Disk are five additional files which are "included" in the main program or in subroutines at the time of compilation. ENB.DAT and INDEX.DAT are for inclusion in XCOM, HASH1.DAT and HASH2.DAT in FORM, and ATWTS.DAT in XCOM and FORM.

5. How to Run the XCOM Program

If the program is to be run using only floppy disks, the Program Disk should be inserted into drive A. After the appearance of the A> prompt, the program can be started by entering "XCOM".

If the program is to be run from a hard disk, it is recommended that a special subdirectory be created for running XCOM. First, the user should copy the file XCOM.EXE from the Program Disk and the data files MDAT.001, MDAT.002, ..., MDAT.100 from the Database Disk into the special directory. After the special directory is made the current directory, the program can be started by entering XCOM.

From this point on, the program proceeds interactively. The user must respond to prompts (indicated by −−>) by entering requested input data or by making choices from various options. The requested information pertains to the name and characterization of the substance of interest, the desired set of energies at which cross sections are to be computed, and the form of the output.

The prompts are largely self−explanatory. In order to indicate to the user what to expect, we show in this report a record of prompts and responses that appeared on the monitor screen in three sample runs of XCOM, for an element (lead) in Appendix A, for a compound (calcium tungstate) in Appendix B, and for a mixture (pyrex glass) in Appendix C. The XCOM program could probably be run without further explanations. Additional information is provided in the remainder of this Section, which will help the user to formulate his responses to the prompts.

5.1. Name of Substance.

The name can be freely chosen, may include imbedded blanks, and must consist of no more than 72 characters. The name will appear on the top of the output table.

5.2. Elements, Compounds and Mixtures.

The substance for which cross sections are to be computed can be designated to be an element, compound or mixture. Elements can optionally be indicated by their atomic number, or by their chemical symbol. These symbols, or chemical formulas for compounds, should be entered in standard chemical notation, with appropriate upper and lower case. However, because of hardware limitations, subscripts must be written on line. For example, the formula for calcium tungstate must be entered as CaWO4.

Substances consisting of molecules with only a single species of atoms can be designated as either as elements or compounds. For example, molecular nitrogen could be treated as an "element" with symbol N, or as a compound with formula N2 (entered as N2).

5.3. Mixtures.

Mixtures are assumed to consist of two or more components, each of which can be either an element or a compound. Whether the mixture is broken

down into "elemental" components or "compound" components is a matter of convenience (depending on the readily available information), but does not change the results.

The user must indicate how many components there are in the mixture, and must specify the chemical symbol or formula, as well as the fraction by weight, for each component, as prompted. The program then uses these input data to compute the fractions by weight of for the individual atomic constituents, as well as the sum of these fractions. This information is displayed on the monitor screen. The input data might be faulty in the sense that the sum of the fractions by weight does not add up to unity. In this case the user is given two choices: 1) The input data can be "accepted", in which case the program renormalizes all of the fractions by weight so that they add up to unity; 2) Another set of fractions by weight for the mixture can be entered.

5.4. Quantities and Units.

For elements, the user is given three choices: 1) the output can consist of cross sections for individual processes, and total cross sections, in units of barns/atom, where 1 barn =10E−24 cm2; 2) the output can consist of cross sections for individual processes, in barns/atom, and mass attenuation coefficients, in cm2/g; 3) the output can consist of partial mass interaction coefficients and, total mass attenuation coefficients, in cm2/g. For compounds and mixtures the output always consists of partial mass interaction coefficients, and total attenuation coefficients, in cm2/g.

5.5. Energy List.

The user can 1) limit the output to the standard energy grid, 2) add to the standard grid selected energies of his choice, or 3) request output only for the set of energies selected by him. In case 2) the additional energies are merged into the standard energy grid according to magnitude. In case 3), the energies will appear in the output table exactly in the sequence in which they were entered by the user.

If additional energies are entered by the user, this can be done, optionally, either from the keyboard, or from a previously prepared input file. This file (stored in any desired directory on a floppy or hard disk) should contain, as first item, the number of additional energies, and then a list of energies, which items separated by blank spaces.

5.6. Database Input Data

The program will prompt the user as to the location of the file containing the database files. The user can request that these data be read from a floppy disk drives (A or B), or from the current directory in the hard disk. Even when the program is run from the special directory on the hard disk, the data can still come from drives A or B. If the data are to come from the hard disk, they must have been previously stored in the special directory, i.e., the current directory from which the XCOM run was started.

5.7. Output Table

The user is asked by a prompt where the file with the cross section table is to be stored. The file specification can include the letter of the drive, the subdirectory, and the file name. If the current directory on a hard disk is to be used, only the file name need be supplied. If the user wants to see the output table only on the monitor screen, the output file should be designated as "CON". If the user wants neither to inspect nor to save the output table (because only the output arrays discussed in section 5.8 are wanted), the output file should be designated as "NUL".

On the top of each page of the table the name of the substance is given, followed by a listing of the atomic numbers and fractions by weight of the atomic constituents. The main body of the table is supplied with enough headings to be self−explanatory. This left−most column gives the designa−tions of the absorption edges (K, L1, L2, L3, M1, M2,..) as well as the

atomic number Z of the pertinent atomic constituent. Data for energies immediately below and above each edge, are given on two lines separated by a blank line. It should be noted that the standard energy grid automatically includes at least one other energy between any two successive absorption edges. For materials of low atomic number, there are no absorption edges above 1 keV, and the column indicating the names of edges is absent.

Typical output tables are shown in Table 1 (for an element, lead), in Table 2 (for a compound, calcium tungstate) and in Table 3 (for a mixture, pyrex glass: 0.807 SiO_2, 0.129 B_2O_3, 0.038 Na_2O, 0.022 Al_2O_3, and 0.004 K_2O by weight). On the top of each page, the name of the substance is given, followed by a listing of the atomic numbers and fractions by weight of the atomic constituents. Fig. 1 shows some of the results from Table 2, namely, the total mass attenuation coefficient plotted as a function of the photon energy.

5.8 Additional Output Arrays

The cross section tables described in Section 5.7 are directly comparable in format to printed tables found in the literature, and are most convenient for visual inspection of the data. If these data are to be used in subsequent computer calculations, the appropriate cross section arrays must be extracted for the tables. XCOM provides an option which facilitates this task.

After the production of the cross section table is completed, the program prompts the user to indicate whether additional output in the form of arrays of selected quantities is desired. If the answer is affirmative, a selection menu is presented. The arrays which can be selected correspond to the columns in the cross section table. After each selection, this menu is presented again.

The user is also asked to provide the name of the file in which the additional arrays are to be stored. At the beginning of this file, preceding the arrays, the following information is stored. The first record consists of the name of the substance. The second record gives the number of atomic constituents, the third contains a list of atomic numbers of the constituents and the fourth a list of fractions by weight.

The fifth record gives the number of sub-arrays into which each array is divided, and the sixth contains the lengths of all successive sub-arrays. Each sub-array contains data for all energies between two adjacent absorption edges. This partitioning facilitates the setting up of interpolation schemes in which interpolation across absorption edges is avoided.

Subsequent records contain, for each of the quantities selected, an identifier (such as "energy list," "total attenuation coefficient") followed by one or more sub-arrays.

Even though the arrangement of the file, as described above, may appear somewhat complicated, it can easily be understood by comparison with the corresponding output table. A typical set of output arrays, consisting of photon energies and total mass attenuation coefficients for calcium tungstate, is given Table 4. These arrays are the same as the data in columns 2 and 7 in Table 2, and were used to produce the plot in Fig. 1.

Acknowledgement.

This work was supported by the NBS Office of Standard Reference Data, and by the U.S. Department of Energy (OHER).

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#XOP on-line help file: xcrosssec.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:14 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/xcrosssec.pro -
----

================================  XCrossSec     ============================

 XCrossSec is a widget based graphical interface to calculate Photon-Atom
 Cross Sections, Mass Absorption Coefficients amd Liner Absorption Coeff.
 for elements, compounds and mixtures.
 The data are taken from the DABAX data base.
 It uses the following DABAX files:
    CrossSec_*.dat  (for tabulated Cross Sections.
                     Presently *={EPDL,XCOM,McMaster}
    Compounds.dat   (for mixture and compounds list)
    AtomicConstants.dat (for atomic Mass and Density)

 Possible calculations:
        Cross Section [barn/atom]
        Cross Section [cm^2]
        Mass Absorption Coefficient [cm^2/g]
        Linear Absorption Coefficient [cm^-1]
        Energy Transfer (Linear and Mass) Coeff [cm^2/g,cm^-1]: This
         option is only allowed by using the DABAX file
         CrossSec_EDPL.dat, where these values are tabulated.
         See doc on this file for additional information.


 CUSTOMIZATION OF XCROSSSEC INPUT PARAMETERS:
  -If you want to add(remove) another CrossSec_* file, just add(remove) it
        in any(all) directory of $DABAX_PATH. Note that the CrossSec
        files containing all the partial cross section (the ones used
        here) only have a single underscore (_).
 -If you want to modify the mixture table  list, do the following:
     > a) copy the Compounds.dat DABAX file to a given directory
        (e.g., current directory ".")
     > b) Modify this file to add/remove/change the entries.
     > c) Redefine $DABAX_PATH to include your new directoty:
        setenv  DABAX_PATH = .:$DABAX_PATH
     > d) Restart the application.


 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    XCrossSec input parameters: This option allows to save the current
                parameters to a file for later loading. It also allows
                to save the current parameters as defaults for being
                used when the application is initialized. In the last
                case, the file is named "application".xop (where
                "application " is the name of the current XOP
                application) and is written in the directory pointed
                by the XOP_DEFAULTS_DIR environment variable (which
                must be set). The parameter file is ASCII and can be
                read and edited with care.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                The same result is obtained pressing the "Set Parameters"
                button in the main XCrossSec window.
               Please refer to the information under the HELP
                button for a complete description of the parameters. After
                pressing the ACCEPT button, xcrosssec starts running and
                creates a graphic window with the results.
  Set Defaults: Sets the default parameters.

  Help:   Shows the XCrossSec help (this text).
```

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/03-01-10

#XOP on-line help file: xcrosssec_par.txt

This is a description of the input parameters for xCrossSec

datasets:
Select a DABAX file from where the Photon-Atom Cross section will be read. The "all" option is also available, and in this case all datasets are used (useful for comparisons).

material: Select the desired material type. Three options are available:
a) Element(formula) calculation for a single element.
b) Mixture(formula) calculation for a compound or a mixture. The user defines the mixture formula.
The syntaxis is the following: string with the chemical formula of the compound(s) with their weight fraction between parenthesis.
Examples:
H20
SiO2(0.807)B2O3(0.129)Na2O(0.038)Al2O3(0.022)K2O(0.004)
H2O(0.99)Cl2(0.01)
H(0.11189834)O(0.88810166)
c) Mixture(table) calculation for a compound or a mixture defined in the included mixture-table (from dabax file Compounds.dat)

table: Compound table, only available if the c) option in material is chosen.

formula: The element or compound or mixture formula, depending the "material" selection.

calculate: type the calculation magnitude. The typed word will be compared with the magnitude name in the DABAX file, and if they match, the corresponding data are loaded.
The "all" option is also available, and in this case all datasets are used (useful for comparisons).

Energy [eV] grid: the abscissas values for the calculations. Two options are available:
a) Standard, which is the energy grid defined in the DABAX file read in first place.
b) User-defined, with the parameters described below.
c) Single-value, with the energy to be entered in "Starting Energy [eV]" box.

Stating Energy [eV]: the initial energy value (only available if either b) or c) is chosen in the "Energy [eV] grid" entry.

To: the last energy value (only available if b) is chosen in the "Energy [eV] grid" entry.

Number of points: the number of energy points (only available if b) is chosen in the "sin_theta/lambda grid" entry.

Units: the units in which the Cross Sections are presented

#XOP on-line help file: xcrystal.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:14 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/optics/xcrystal.pro ----

==========   xcrystal   ==========

Xcrystal is a widget based graphical interface to calculate diffraction profiles of perfect and mosaic crystals. It allows Bragg and Laue geometries and (in the case of perfect crystals) diffracted and transmitted intensity calculations. The diffracted intensity can be calculated as a function of either rock angle or photon energy. It uses the DABAX database to define the crystal structure and to retrieve the scattering factors to build the crystal structure factors.

It interfaces diff_pat, a computer program written by M. Sanchez del Rio (srio@esrf.fr) derived from the SHADOW application bragg.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
Xcrystal input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main XCrystal window. Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, diff_pat starts running.
Set Defaults: Sets the default parameters.

Show: Display results
Diffraction Curve: starts a graphical window with the calculation results.
Crystal Parameters: shows output parameters of the calculation.
Crystallographic Parameters: shows numerical values used to build the crystal structure factor.

Help: Shows the xcrystal help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations with the xcrystal_bent aplication should also cite:

M. Sanchez del Rio, C. Ferrero and V. Mocella. "Computer simulations of bent perfect crystal diffraction profiles" SPIE proceedings vol. 3151, pp.312-323, 1997.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xcrystal_bent.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:14 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/optics/xcrystal_bent.pro -----

==========   Xcrystal_bent   ==========

Xcrystal_bent is a common widget based graphical interface to different codes that perform curved crystal diffraction calculations.

The idea is to perform bent crystal calculations with different modules (computer codes) using the same interface. The different modules use different theories. The initial considered theories are:

1) Lamellar theory.
2) Penning Polder theory.
3) Takagi-Taupin theory.
In addition, and for comparison purposes, a module to calculate flat perfect crystals, based on the Zachariasen's theory has been included. For FLAT crystals calculations it is recommended to use the xcrystal application in XOP>

Plase note that:
The Penning-Polder model is only available for LAUE crystals
The Takagi-Taupin model is under testing for BRAGG crystals, and it may not produce correct results.

XCrystal_bent uses the codes crystal_za (Zachariasen), crystal_ml (Multi-lamellar) crystal_pp (Penning-Polder) and crystal_tt (Takagi-Taupin).

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
xcrystal_bent input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main crystal_bent window. Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, the corresponding code starts running.
Set Defaults: Sets the default parameters.
Takagi-Taupin specific parameters: two items (Set Parameters & Set Defaults) allows to define the specific parameters for Takagi-Taupin calculations. They are placed in different windows to allow a too complicated main window.

Show: Plot, View or Print the results.
Diffraction Curves: display calculated diffraction curves.
Bent Crystal Parameters: shows numerical parameters of the calculations.
Crystallographic Parameters: shows numerical parameters used for the calculation of the crystal structure factor.
Takagi-Taupin: Some specific outputs only available if using the Takagi-Taupin theory.

Integration Network: Shows the integration network with the
electric field corresponding to y=0.
This option is only available when the calculations is
requested in the TAKAGI-TAUPIN/SET PARAMETERS option.
All Reflectivity Curves: Shows an array of diffraction
profiles corresponding, each one, to one knot in the
incident surface.
This option is useful to check that the "window" parameter
is large enough to avoid border effects in the main (central)
diffraction profile.
This option is only available when the calculations is
requested in the TAKAGI-TAUPIN/SET PARAMETERS option.

Help: Shows the xcrystal_bent help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations with the xcrystal_bent aplication
should also cite:
M. Sanchez del Rio, C. Ferrero and V. Mocella.
"Computer simulations of bent perfect crystal diffraction profiles"
SPIE proceedings vol. 3151, pp.312-323, 1997.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xcrystal_bent_par.txt

This is a description of the input parameters for xcrystal_bent

DABAX f0 file:
Select a DABAX file from where the f0 component of the structure factor will be read.

DABAX f1f2 file: Select a DABAX file from where the f1f2 components of the structure factor will be read.

Crystal: Select a crystal from this list of crystals.

h Miller index: obvious
k Miller index: obvious
l Miller index: obvious

Include absorption: Recommended to select *ALWAYS* Yes.

Temperature factor: Three possibilites:
1) Enter the exp(-M) value (a positive value between 0 and 1)
2) Enter the absolute temperatute in Kelvin, WITH A MINUS SIGN.
The minus sign tells to the code that the number entered refers to a temperature and not to the full debye-waller exp(-M) factor. The minus sign will not be considered for the numerial calculations.
In this case, the Debye-Waller factor is calculated as a function of the temperature, using a well-known approximation as a function of sin(theta/lambda)=1/(2d), temperature, atomic mass and Debye-temperature. In the case of crystal structures with more that one atomic sites, an independent Debye-Waller factor is calculated for each atomic site and then putting them together by averaging the M's. Values for atomic mass and Debye temperatures are obtained from the DABAX file AtomicConstants.dat. For more info, see the documentation in the function DebyeWaller.pro
3) Enter a question mark (?).
In this case, the code will perform the calculation as in point 2), but it will pop-up a window that will permit to modify the Debye-Waller ingredients (i.e., the sin(theta/lambda)=1/(2d) ratio, temperatute, atomic mass and Debye temperature).
In the case of crystal structures with several atomic types, several values of atomic mass and Debye temperature should be entered.
The default values are taken from the DABAX file AtomicConstants.dat.
The interest of this option is to allow the user to "improve" the default value of the temperature factor, which is mostly "structure" dependent rather than dependent on the atomic types. For example, in the case of AlphaQuartz (SiO2), The Debye temperature of the oxygen is not defined by default in the AtomicConstants.dat DABAX file because oxigen does not exist in crystalline state. Therefore the averaged value seems not realistic.
This option allows to customize the Debye temperatures from default (note that values of Debye temperature found in bibliography change significatively from one reference to another) and also allows to enter average values of atomic mass and Debye temperature by entering identical values foe all atomic sites.
Note that if values are changed in this window, they are not saved for further runs, nor saved to input files like xcrystal_bent.xop.

Calculation Theory: Select the desired theoretical model for the bent crystal calculations. The options here are initialized in the $XOP_HOME/data/crystal_bent_theories.dat. Some models have limitations that must be kept in mind, because the application does not tell the user about a wrong use.
For example, Zachariasen theory is only for FLAT crystals (so the bent radius and Poisson ration values are ignored) and Penning-Polder theory is only for crystals in LAUE geometry.

Geometry: Select between LAUE or BRAGG.

Min Y value: min value for the rock angle scanning in function of the
Y variable.

Max Y value: max value for the rock angle scanning in function of the
Y variable.

Number of points: the number of points in Y.

Photon EnergY [eV]: The photon energy in eV

Asymmetry Angle [deg]: the angle between the Bragg planes and the crystal
surface. It is 0.0 for the symmetrical Bragg case and 90.0 for
the symmetrical Laue case.

Polarization: use Sigma for polarization factor P=1.
Pi for P=cos(2*theta_bragg)
Total for non-polarized incident ligth P=0.5(1+cos(2*theta_bragg)).

Radius of Curvature [m]: The crystal radius in meters.

Crystal Thickness [mm]: the crystal thickness in mm

Poisson Ratio: The Poisson ration (elastic constant) for the selected crystal.
Plase note that only homogeneous materials are considered in the
deformation model.

#XOP on-line help file: xcrystal_bent_tt_par.txt

The parameters in this window are specific for the Takagi-Taupin (TT) codes of the xcrystal_bent application.

They are ignored for the non-TT models.

Window [microns]:
Set here the number of microns of "window".
"Window" is the dimension of the integration network (Borrmann fan) along the crystal surface.
Other special values are accepted:
0 = use the default value calculated internally by cryst_tt
-X = means X times the default value. For example -0.2 means that window is set to 20% of the default value.

Step [microns]:
Set here the number of microns of "step".
"Step" is the dimension of a step of the the integration network (Borrmann fan) in the perpendicular direction of the crystal surface.
Other special values are accepted:
0 = use the default value calculated internally by cryst_tt
-X = means X times the default value. For example -2 means that step is twice default value.

Write file with network?
Allows to write a file (cryst_tt.net) containing the network and the electric field on that network.
It can be siaplayed with Show/Takagi-Tapin/Integration Network option.

Write file with all diff profiles?
Allows to write a file (cryst_tt.all) containing the diffraction profiles in all the knots of the intersection between the integration network with the exit surface.
It can be siaplayed with Show/Takagi-Tapin/All reflectivity curves option.

RECOMMENDATIONS:

The network dimension incrteases when "window" increases, and also increases when "sted" decreases. A carefull definition of these parameters is essential. A large network can affect in an extremely long calculation time. The calculation time can be estimated from the text displayed in the spawned log screen. It is not possible to abort the calculations from the interface. Long calculation may be aborted by aborting the XOP session. Under Unix the process can be aborted from another terminal window, by locating the process id (using ps -u username | grep cryst) and killing such a process number (using kill). Under Windows, the task can be aborted from the window that appears when pressing <Ctl><Alt><Del> at the same time.

The diffraction profile is taken from the central point of the "window". If "window" is too small, border effects can affect this main diffraction profile. In order to check if the border effects are important at the central point, one can display all thediffraction profiles (in all the knot points) using the option: Show/Takagi-Tapin/All reflectivity curves.

The "elem" should be small enough to avoid spurious oscillations and to be able of following the phase of the diffracted beam. For example, thin crystals may present Pendelloesung oscillations which period is completely wrong is "elem" is not correctly set.

They are not recipes for such values. The defaults set by cryst_tt are calculated from the Pendelloesung length (l_pen):
For Bragg/flat crystals:
window = l_pen*400.0
elem = window/100.0

```
For Bragg/bent crystals:
  window = l_pen*120.0
  elem = window/50.0
For Laue crystals:
  window = 3.0*(thickness+tan(thetab+alpha))
  elem=window/300.0
```

#XOP on-line help file: xcrystal_par.txt

This is a description of the input parameters for xcrystal

DABAX f0 FILE:
Select a DABAX file from where the f0 component of the structure factor will be read.

DABAX f1f2 FILE: Select a DABAX file from where the f1f2 components of the structure factor will be read.

CRYSTAL: Select a crystal from this list of crystals.

h MILLER INDEX: obvious
k MILLER INDEX: obvious
l MILLER INDEX: obvious

TEMPERATURE FACTOR: Three possibilites:
1) Enter the exp(-M) value (a positive value between 0 and 1)
2) Enter the absolute temperatute in Kelvin, WITH A MINUS SIGN.
The minus sign tells to the code that the number entered refers to a temperature and not to the full debye-waller exp(-M) factor. The minus sign will not be considered for the numerial calculations.
In this case, the Debye-Waller factor is calculated as a function of the temperature, using a well-known approximation as a function of sin(theta/lambda)=1/(2d), temperature, atomic mass and Debye-temperature. In the case of crystal structures with more that one atomic sites, an independent Debye-Waller factor is calculated for each atomic site and then putting them together by averaging the M's. Values for atomic mass and Debye temperatures are obtained from the DABAX file AtomicConstants.dat. For more info, see the documentation in the function DebyeWaller.pro
3) Enter a question mark (?).
In this case, the code will perform the calculation as in point 2), but it will pop-up a window that will permit to modify the Debye-Waller ingredients (i.e., the sin(theta/lambda)=1/(2d) ratio, temperatute, atomic mass and Debye temperature).
In the case of crystal structures with several atomic types, several values of atomic mass and Debye temperature should be entered.
The default values are taken from the DABAX file AtomicConstants.dat.
The interest of this option is to allow the user to "improve" the default value of the temperature factor, which is mostly "structure" dependent rather than dependent on the atomic types. For example, in the case of AlphaQuartz (SiO2), The Debye temperature of the oxygen is not defined by default in the AtomicConstants.dat DABAX file because oxigen does not exist in crystalline state. Therefore the averaged value seems not realistic.
This option allows to customize the Debye temperatures from default (note that values of Debye temperature found in bibliography change significatively from one reference to another) and also allows to enter average values of atomic mass and Debye temperature by entering identical values foe all atomic sites.
Note that if values are changed in this window, they are not saved for further runs, nor saved to input files like xcrystal.xop.

MOSAIC CRYSTAL: Select YES when you want "mosaic crystal", otherwise "perfect crystal" is set.

GEOMETRY: select one of the four cases combining Laue and Bragg cases for either diffracted or transmitted beam. Note that the transmitted intensity is not implemented for mosaic crystals.

SCAN: The scanned variable for the plot. Angular and Energy scans are allowed. The angular variable can be: Theta, when absolute angle is wanted; Th-ThBragg(corrected) or angular scan with zero at the bragg angle corrected for refraction; Th-ThBragg or angular

scan with zero at the bragg angle; and y is dimensionless angular variable defined by (for instance) in the Zachariasen book.
In the case of angular scans the unit can be set, except in the case of y. Energy is always in eV.

SCAN UNITS: angular units, if angular scan is set.

MIN SCAN VALUE: min value for the scanning variable.

MAX SCAN VALUE: max value for the scanning variable.

SCAN POINTS: the number of scanning points.

FIX VALUE (E[eV]) OR Theta[deg]): Place here either the energy value of the monochromatic incident photon beam (when angular scan is selected) or the grazing angle [in degrees] when a energy scan is wanted.
In the case of energy scan, the program can calculate automatically the theta angle if one inputs the energy. If this option is selected, enter the Energy with a minus sign in this box.

ASYMMETRY ANGLE [deg]: the angle between the Bragg planes and the crystal surface. It is 0.0 for the symmetrical Bragg case and 90.0 for the symmetrical Laue case.
This input is not present when using Mosaic crystals, which are always symmetrical.

CRYSTAL THICKNESS [cm]: the crystal thickness in cm

MOSAICITY [deg fwhm]: The mosaicirty of the mosaic crystal (if selected).

#XOP on-line help file: xf0.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:14 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/xf0.pro -----
================================   xF0   ================================

xf0 is a widget based graphical interface to calculate Elastic
Photon-Atom Scattering versus x=sin(theta/2)/lambda.

The data are taken from the DABAX data base.
It uses the following DABAX files:
  f0_*.dat (for f0 values)

  Compounds.dat   (for mixture and compounds list)

CUSTOMIZATION OF XF0 DABAX PARAMETERS:
 -If you want to add(remove) another f0_* file, just add(remove) it
  in any(all) directory of $DABAX_PATH.
-If you want to modify the mixture table list, do the following:
    a) copy the Compounds.dat DABAX file to a given directory
       (e.g., current directory ".")
    b) Modify this file to add/remove/change the entries.
    c) Redefine $DABAX_PATH to include your new directoty:
       setenv DABAX_PATH = .:$DABAX_PATH
    d) Restart the application.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

 File:
   XF0 input parameters: This option allows to save the current
               parameters to a file for later loading. It also allows
               to save the current parameters as defaults for being
               used when the application is initialized. In the last
               case, the file is named "application".xop (where
               "application " is the name of the current XOP
               application) and is written in the directory pointed
               by the XOP_DEFAULTS_DIR environment variable (which
               must be set). The parameter file is ASCII and can be
               read and edited with care.
 Quit: to exit from the program

Set_Parameters:
 Set Parameters: to define the parameters for the calculation.
               The same result is obtained pressing the "Set Parameters"
               button in the main XF0 window.
               After pressing the ACCEPT button, F0 starts running and
               displays a graphical window with the results.

 Help: Shows the Xf0 help (this text).

CREDITS:
       Published calculations made with XOP should refer:

         M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
         SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/03-02-04

#XOP on-line help file: xf0_par.txt

This is a description of the input parameters for xf0

datasets:
Select a DABAX file from where the f0 scattering factors
will be read. The "all" option is also available, and
in this case all datasets are used (useful for comparisons).

material: Select the desired material type. Three options are available:
a) Element(formula) calculation for a single element.
b) Mixture(formula) calculation for a compound or a mixture. The user
defines the mixture formula.
The syntaxis is the following: string with the chemical
formula of the compound(s) with their weight fraction between
parenthesis.
Examples:
H20
SiO2(0.807)B2O3(0.129)Na2O(0.038)Al2O3(0.022)K2O(0.004)
H2O(0.99)Cl2(0.01)
H(0.11189834)O(0.88810166)
c) Mixture(table) calculation for a compound or a mixture defined
in the included mixture-table (from dabax file Compounds.dat)

table: Compound table, only available if the c) option in material is chosen.

formula: The element or compound or mixture formula, depending the "material"
selection.

sin_theta/lambda [A**(-1)] grid: the abscissas values for the calculations. Two
options are available:
a) Standard, 515 points in the [0,8] interval.
b) User-defined, with the parameters described below.

Form : the initial abscissa value (only available if b) is chosen)

To: the last abscissas value (only available if b) is chosen)

Number of points: the number of energy points (only available if b) is
chosen in the "sin_theta/lambda grid" entry.

#XOP on-line help file: xf1f2.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:14 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/xf1f2.pro -----

 ================================ xf1f2   ============================

 xf1f2 is a widget based graphical interface to calculate Elastic
 Anomalous Photon-Atom Scattering, and their derived parameters
 (refraction index, photoelectric absorption, reflectivity).

 The data are taken from the DABAX data base.

 Possible calculations:
              f1
              f2
              delta [n=1-delta-i beta]
              beta [n=1-delta-i beta]
              Photoelectric linear abs coeff (mu [cm^-1)]
              Photoelectric mass abs coeff (mu [cm^2/g)]
              Photoelectric Cross Section [barns]
              s-pol reflectivity
              p-pol reflectivity
              unpolarized reflectivity

 CUSTOMIZATION OF Xf1f2 DABAX INPUT PARAMETERS:
  -If you want to add(remove) another f1f2* file, just add(remove) it
   in any(all) directory of $DABAX_PATH.
 -If you want to modify the mixture table list, do the following:
     a) copy the Compounds.dat DABAX file to a given directory
        (e.g., current directory ".")
     b) Modify this file to add/remove/change the entries.
     c) Redefine $DABAX_PATH to include your new directoty:
        setenv DABAX_PATH = .:$DABAX_PATH
     d) Restart the application.

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    Xf1f2 input parameters: This option allows to save the current
                 parameters to a file for later loading. It also allows
                 to save the current parameters as defaults for being
                 used when the application is initialized. In the last
                 case, the file is named "application".xop (where
                 "application " is the name of the current XOP
                 application) and is written in the directory pointed
                 by the XOP_DEFAULTS_DIR environment variable (which
                 must be set). The parameter file is ASCII and can be
                 read and edited with care.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                 The same result is obtained pressing the "Set Parameters"
                 button in the main Xf1f2 window.
                Please refer to the information under the HELP
                 button for a complete description of the parameters. After
                 pressing the ACCEPT button, xf1f2 start running and
                 presents a graphic display with results.
  Set Defaults: Sets the default parameters.

  Help: Shows the xf1f2 help (this text).

 COPYRIGHT:
        xf1f2 belongs to XOP package and it is distributed within XOP.
        PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xf1f2_par.txt

This is a description of the input parameters for xf1f2

datasets:
Select a DABAX file from where the f1f2 scattering factors will be read. The "all" option is also available, and in this case all datasets are used (useful for comparisons).

material: Select the desired material type. Three options are available:
a) Element(formula) calculation for a single element.
b) Mixture(formula) calculation for a compound or a mixture. The user defines the mixture formula.
The syntaxis is the following: string with the chemical formula of the compound(s) with their weight fraction between parenthesis.
Examples:
H2O
SiO2(0.807)B2O3(0.129)Na2O(0.038)Al2O3(0.022)K2O(0.004)
H2O(0.99)Cl2(0.01)
H(0.11189834)O(0.88810166)
c) Mixture(table) calculation for a compound or a mixture defined in the included mixture-table (from dabax file Compounds.dat)

table: Compound table, only available if the c) option in material is chosen.

formula: The element or compound or mixture formula, depending the "material" selection.

density: The mixture density in the case that option b) has been selected.

calculate: select the calculation magnitude. The "all" option is also available, and in this case all datasets are used (useful for comparisons). The "all" option here is incompatible with the "all" option in the "datasets" entry.

Energy [eV] grid: the abscissas values for the calculations. Two options are available:
a) Standard, 100 points in the [0,3] interval.
b) User-defined, with the parameters described below.
c) Single-value, with the energy to be entered in "Starting Energy [eV]" box.

Stating Energy [eV]: the initial energy value (only available if either b) or c) is chosen in the "Energy [eV] grid" entry.

To: the last energy value (only available if b) is chosen in the "Energy [eV] grid" entry.

Number of points: the number of energy points (only available if b) is chosen in the "sin_theta/lambda grid" entry.

Grazing angle: the surface grazing angle (only available when "reflectivity" calculations are set in "Calculate" entry. Two options are available:
a) Single-value, for calculations of Reflectivity versus energy.
b) User-defined, for calculations of Reflectivity versus angle, or reflectivity versus both angle and energy (2D plot).

Roughness rms [A]: The surface RMS roughness (only available when "reflectivity" calculations are set in "Calculate" entry.

Stating Graz angle [mrad]: the grazing angle (when single-value is set) or the initial grazing angle value (only available for reflectivity calculations).

To: the last grazing angle value (only available if both b) is chosen in the "Grazing angle" entry and for reflectivity calculations).

Number of angular points: the number of angle points (only available if both b) is chosen in the "Grazing angle" entry and for reflectivity calculations).

#XOP on-line help file: xfh.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:15 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/dabax/xfh.pro -----

================================ xfh ================================

 XFH is a widget based graphical interface to calculate structure
 factor of crystals.

 The data are taken from the DABAX data base.

 It access the following DABAX files:
        CrystalStructures.dat
        CrystalCell.dat
        f1f2_*.dat
        f0_CromerMann.dat,f0_CromerMann_old1968.dat,f0_WaasKirf.dat

 CUSTOMIZATION OF XFH INPUT PARAMETERS:
  -If you want to add(remove) another f1f2* file, just add(remove) it
   in any(all) directory of $DABAX_PATH.
  -If you want to add(remove) another f0 file, follow the inscructions
        given before.
  -If you want to modify the crystal list, do the following:
        a) copy the CrystalStructures.dat and CrystalCell.dat files to
           a given directory (i.e. current directory ".")
        b) Modify these files to add/remove/change the entries. Both
            files must have the same entries (or "scans").
        c) Redefine $DABAX_PATH to include your new directoty:
           setenv DABAX_PATH = .:$DABAX_PATH
        d) Restart the application.

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    Xfh input parameters: This option allows to save the current
                 parameters to a file for later loading. It also allows
                 to save the current parameters as defaults for being
                 used when the application is initialized. In the last
                 case, the file is named "application".xop (where
                 "application " is the name of the current XOP
                 application) and is written in the directory pointed
                 by the XOP_DEFAULTS_DIR environment variable (which
                 must be set). The parameter file is ASCII and can be
                 read and edited with care.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                 The same result is obtained pressing the "Set Parameters"
                 button in the main Xfh window.
                Please refer to the information under the HELP
                 button for a complete description of the parameters. After
                 pressing the ACCEPT button, xfh starts running and
                 creates a graphical window with the results.
  Set Defaults: Sets the default parameters.

  Show: Diaplay results
    Plot crystal parameters: performs a plot of the energy-dependent parameters
                 (this option os only available for a number of energy points
                  nonequal to one)
    Show crystal parameters: Show text information of the crystal parameters
    Show crystallographic parameters: Show parameters used to build the
                 structure factor.
  Help: Shows the xfh help (this text).

 COPYRIGHT:

xfh belongs to XOP package and it is distributed within XOP.
PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/2003-01-10

#XOP on-line help file: xfh_par.txt

This is a description of the input parameters for xfh

DABAX f0 FILE:
Select a DABAX file from where the f0 component of the structure factor will be read.

DABAX f1f2 FILE: Select a DABAX file from where the f1f2 components of the structure factor will be read.

CRYSTAL: Select a crystal from this list of crystals.

h MILLER INDEX: obvious
k MILLER INDEX: obvious
l MILLER INDEX: obvious

TEMPERATURE FACTOR: Three possibilites:
1) Enter the exp(-M) value (a positive value between 0 and 1)
2) Enter the absolute temperatute in Kelvin, WITH A MINUS SIGN.
The minus sign tells to the code that the number entered refers to a temperature and not to the full debye-waller exp(-M) factor. The minus sign will not be considered for the numerial calculations.
In this case, the Debye-Waller factor is calculated as a function of the temperature, using a well-known approximation as a function of sin(theta/lambda)=1/(2d), temperature, atomic mass and Debye-temperature. In the case of crystal structures with more that one atomic sites, an independent Debye-Waller factor is calculated for each atomic site and then putting them together by averaging the M's. Values for atomic mass and Debye temperatures are obtained from the DABAX file AtomicConstants.dat. For more info, see the documentation in the function DebyeWaller.pro
3) Enter a question mark (?).
In this case, the code will perform the calculation as in point 2), but it will pop-up a window that will permit to modify the Debye-Waller ingredients (i.e., the sin(theta/lambda)=1/(2d) ratio, temperatute, atomic mass and Debye temperature).
In the case of crystal structures with several atomic types, several values of atomic mass and Debye temperature should be entered.
The default values are taken from the DABAX file AtomicConstants.dat.
The interest of this option is to allow the user to "improve" the default value of the temperature factor, which is mostly "structure" dependent rather than dependent on the atomic types. For example, in the case of AlphaQuartz (SiO2), The Debye temperature of the oxygen is not defined by default in the AtomicConstants.dat DABAX file because oxigen does not exist in crystalline state. Therefore the averaged value seems not realistic.
This option allows to customize the Debye temperatures from default (note that values of Debye temperature found in bibliography change significatively from one reference to another) and also allows to enter average values of atomic mass and Debye temperature by entering identical values foe all atomic sites.
Note that if values are changed in this window, they are not saved for further runs, nor saved to input files like xcrystal.xop.

FROM ENERGY [eV]: the starting photon energy for the calculation.

TO ENERGY [eV]: the starting photon energy for the calculation.

NUMBER OF POINTS: the number of points for the energy grid.
If set to 1, only the minimum energy point is calculated.

#XOP on-line help file: xinpro.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:15 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/optics/xinpro.pro ---
--

============================ Xinpro ===================================

Xinpro is a widget based graphical interface to calculate perfect crystal reflectivity profiles.

It interfaced the inpro (INtrinsic PROfiles) code. Inpro calculates the diffracted and transmitted profiles in reflection (Bragg) and transmission (Laue) geometries for plane perfect crystals.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Xinpro input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main Xinpro window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, inpro starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Diffraction curves: Plots the inpro results.
  parameters: Displays some outputs from inpro.dat

Help: Shows the Xinpro help (this text).

CREDITS:
      Published calculations made with XOP should refer:

        M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
        SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xinpro_par.txt

Input parameters for xinpro:
==========

Crystal material: Select a crystal from this list of crystals.

Calculation Mode: select between BRAGG/LAUE in REFLECTION/TRANSMISSION.

Energy [eV]: The photon energy.

Miller index h: obvious
Miller index k: obvious
Miller index l: obvious

Asymmetry angle: in degrees. For Laue, the asymmetry angle is defined as the angle between the crystal normal and the bragg plases. For Bragg, this is the angle between the crystal surface and the bragg planes. In other works, for Bragg-symmetrical alpha=0 a,d for Laue symmetrical alpha=0.

Crystal thickness [microns]

Crystal temperature [K]: NOTE: due to the Debye-Model parametrization used, T=0K is not valid!

Number of points

Angular limits: Set either automatic or external.

Theta min [arcsec]: The external minimum value of the scanning variable.

Theta max [arcsec]: The external maximum value of the scanning variable.

```
#XOP on-line help file: xloadct.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:15 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/Embedded/RSI-SRC/xloa
dct.pro -----

 NAME:
       XLOADCT
 PURPOSE:
       A graphical interface to the LOADCT user library procedure.
       XLOADCT displays the current color map and provides
       an array of buttons, one per availible predefined color
       table. Using the mouse to press these buttons causes
       the corresponding color map to be loaded.
 CATEGORY:
       Widgets
 CALLING SEQUENCE:
       XLOADCT
 INPUTS:
       None.
 KEYWORDS:
        FILE:   If this keyword is set, the file by the given name is used
                instead of the file colors1.tbl in the IDL directory.  This
                allows multiple IDL users to have their own color table file.
       GROUP = The widget ID of the widget that calls XLoadct.  When
               this ID is specified, a death of the caller results in a
               death of XLoadct
        NCOLORS = number of colors to use.  Use color indices from BOTTOM
                to the smaller of !D.TABLE_SIZE-1 and NCOLORS-1.
                Default = !D.TABLE_SIZE = all available colors.
        BOTTOM = first color index to use. Use color indices from BOTTOM to
                BOTTOM+NCOLORS-1.  Default = 0.
       SILENT - Normally, no informational message is printed when
               a color map is loaded. If this keyword is present and
               zero, this message is printed.
        USE_CURRENT: If set, use the current color tables, regardless of
                the contents of the COMMON block COLORS.
       MODAL:  If set, then XLOADCT runs in "modal" mode, meaning that
               all other widgets are blocked until the user quits XLOADCT.
               A group leader must be specified (via the GROUP keyword)
               for the MODAL keyword to have any effect.   The default
               is to not run in modal mode.
        BLOCK:  Set this keyword to have XMANAGER block when this
                application is registered.  By default the Xmanager
               keyword NO_BLOCK is set to 1 to provide access to the
               command line if active command   line processing is available.
               Note that setting BLOCK for this application will cause
                all widget applications to block, not only this
                application.  For more information see the NO_BLOCK keyword
                to XMANAGER.
       UPDATECALLBACK: Set this keyword to a string containing the name of
               a user-supplied procedure that will be called when the color
               table is updated by XLOADCT.  The procedure may optionally
               accept a keyword called DATA, which will be automatically
               set to the value specified by the optional UPDATECBDATA
               keyword.
       UPDATECBDATA: Set this keyword to a value of any type. It will be
               passed via the DATA keyword to the user-supplied procedure
               specified via the UPDATECALLBACK keyword, if any. If the
               UPDATECBDATA keyword is not set the value accepted by the
               DATA keyword to the procedure specified by UPDATECALLBACK
               will be undefined.

 OUTPUTS:
       None.
 COMMON BLOCKS:
       None.
 SIDE EFFECTS:
       One of the predefined color maps may be loaded.
 RESTRICTIONS:
```

This routine uses the LOADCT user library procedure to
do the actual work.
MODIFICATION HISTORY:
24, August, 1990, Written by AB, RSI.
March 1, 1992 Mark Rivers added Reverse Table to options menu.
7/92, DMS, Added new color tables (allows more than 16).
9/92, ACY, Add FILE keyword.
10/1/96, AB, Removed the PICK_ONE keyword. It was broken for 4 years
without anyone noticing, and the idea doesn't really fit
XLOADCT anymore.
1/10/97, DJC − Fixed color bar display bug, and added "MODAL" keyword.
1/13/96, AB, Improved the saving and restoring of the current
graphics window to prevent other applications from drawing
on this applications windows.
1/17/97, DJC − Moved group_leader keyword from "XManager" to
"WIDGET_BASE". Added check to ignore "MODAL" keyword
if a group leader is not specified.
8/20/98, ACY − Added UPDATECALLBACK and UPDATECBDATA keywords.

#XOP on-line help file: xop_environment.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:15 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/xoplib/xop_environment.pro -----

NAME:
XOP_ENVIRONMENT

PURPOSE:
Presents a window with the XOP environment variables.
Optionally (see edit keyword) allows editing.

CATEGORY:
XOP

CALLING SEQUENCE:
Xop_Environment

INPUTS:

KEYWORD PARAMETERS:
GROUP: The widget ID of the group leader of the widget. If this
keyword is specified, the death of the group leader results in
the death of widgets created by XOP_ENVIRONMENT.
EDIT: If set, allows to edit the parameters

OUTPUTS:
None

SIDE EFFECTS:
Modify environment variables (is edit keyword is set and
changes are typed).

PROCEDURE:
Straightforward.

USE:
It is launched from the main XOP window for debugging and
customization purposes.

EXAMPLES:
Xop_Environment

MODIFICATION HISTORY:
Written by: Manuel Sanchez del Rio (srio@esrf.fr) 98/11/05
99-04-10 srio@esrf.fr adds XOP_ENV and removes HOME. Only resets
variables if user selects "Quit and accept changes".
03-01-07 srio@esrf.fr Added text with description.

#XOP on-line help file: xop_ifc.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:18 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/xoplib/xop_ifc.pro ----

   ========================== xop_ifc   ========================

   xop_ifc is a generic widget based graphical interface.
   It allows to include xop-like interfaces in xop at run time.
   It reads the inputs from a file <application>.ifc which must be
   sitting in the $XOP_IFC directory or alternatively (is $XOP_IFC
   is undefined) in $XOP_HOME/ifc directory.

   See the file $XOP_HOME/ifc/mlayer.ifc as an example of how to write
   these files.

        srio@esrf.fr 97-04-07
       Modification history:
        97-09-12 srio@esrf.fr makes no_block keyword. Adds the option
          state.ifc.run='<none>' to avoid spawning (to be used in
          applications fully written in IDL). Uses $XOP_IFC as a
          directory from where the *.ifc file is read. If $XOP_IFC
          is not set, uses $XOP_HOME/ifc. xop_ifc_run accepts
          now 21 (a0,...,a20) generic variables... Use of sdep.pro
          for getting system dependencies.
        97-11-07 srio@esrf.fr ifc files are in $XOP_HOME/ifc and not
          longer in $XOP_HOME/data.
        97-11-07 srio@esrf.fr fixes a bug when loading/writing files.
        98-11-04 srio@esrf.fr uses Catch.
        98-11-24 srio@esrf.fr changes to new input file system (xop2.0)
        00-07-17 srio@esrf.fr the tags nrows and ncol in the ifc
                structure are now optional. One of them must be set.
        02-05-23 srio@esrf.fr bug fixed: writes to a file the correct
                version (not 1.0). Added optional input ifc to xop_ifc_run

```
#XOP on-line help file: xop_input_run.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:16 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/xoplib/xop_input_run.
pro -----

 NAME:
       XOP_INPUT_RUN

 PURPOSE:
       This procedure reads an XOP input file, extract the application
        name and runs this application with the parameters in the file.

 CATEGORY:
       XOP

 CALLING SEQUENCE:
       Xop_Input_Run, file

 OPTIONAL INPUTS:
        File: the name of the file containg the parameters to be run.
                 (If inputFile is not set, starts the file browser to get it).

 KEYWORD PARAMETERS:
       GROUP:  The widget ID of the group leader of the widget.  If this
               keyword is specified, the death of the group leader results i n
               the death of widgets created by XOP_WD.
        Confirm: Asks for confirmation befor start the run
        _Extra: any other keyword to be passed to Dialog_PaickFile

 OUTPUTS:
       Starts the corresponding XOP application and loads the inputs.

 SIDE EFFECTS:

 PROCEDURE:
       reads the first line in the <application>.xop file
        (i.e. ; xop/xus(v1.9) input file on Thu Dec  3 17:22:34 1998 )
        and extracts the application name (in this case xus).
        Loads the parameters in the <application>.xop file and stores
        them in the application.

 USE:
       To start any XOP application from the Main XOP window (File menu).

 EXAMPLES:
       Xop_Input_run

 MODIFICATION HISTORY:
       Written by:     Manuel Sanchez del Rio (srio@esrf.fr) 98/11/05
```

#XOP on-line help file: xop_macro.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:16 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/util/xop_macro.pro ---

NAME:
	XOP_MACRO
PURPOSE:
	Edits and runs an XOP macro
CATEGORY:
	Widgets.
CALLING SEQUENCE:
	XOP_MACRO [,inCode]
INPUTS:
	inCode: an array of strings with the code to be processed.
KEYWORD_PARAMETERS:
	GROUP: The widget ID of the group leader of the widget.
		If this keyword is specified, the death of the group
		leader results in the death of XOP_MACRO.
	No_Block: If this keyword is set, then it is passed to
		XManager.
	File: name of the file with the code to be loaded (if
		this keyword is set, the inCode variable is not
		considered).
	Title: the window title (Default: XOP_MACRO)

OUTPUTS:
	Open the widget utility.
COMMON BLOCKS:
	None
SIDE EFFECTS:
	If not active, starts Xmanager
RESTRICTIONS:
	Unknown.
PROCEDURE
	Uses xop_macro_compact. See its doc.
MODIFICATION HISTORY:
	Written by Manuel Sanchez del Rio. ESRF. 22 May 2000

```
#XOP on-line help file: xop_wd.txt

----- file created by xop_makedoc on: Fri Mar  7 13:26:16 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/Embedded/RSI-SRC/xop_
wd.pro -----

 NAME:
       XOP_WD

 PURPOSE:
       Changes XOP working directory. XOP working directry is where
       XOP writes temporary files.

 CATEGORY:
       XOP

 CALLING SEQUENCE:
       XOP_WD
 INPUTS:
       None

 KEYWORD PARAMETERS:
      GROUP:  The widget ID of the group leader of the widget.  If this
              keyword is specified, the death of the group leader results in
              the death of widgets created by XOP_WD.
       DEFAULT: When this keyword is set, XOP_WD changes directory to
                the default XOP Working Directory. This directory is
                specified in the XOP_WD environment variable. If the
                XOP_WD environment variable is not set, the XOP Working
                Directory is  %XOP_HOME%\tmp under WINDOWS and .
                (dot=current directory) under UNIX.
                If this keyword is not set, a dialog_pickfile window
                appears to select interactively the Working Directory.

 OUTPUTS:
       None

 SIDE EFFECTS:
       Changes directory using the IDL's cd command.

 PROCEDURE:
       Straightforward.

 USE:
       This procedure is to be used by XOP_INI when starting XOP.
 EXAMPLES:
       xop_cw
       xop_cw,/defaults

 MODIFICATION HISTORY:
       Written by:     Manuel Sanchez del Rio (srio@esrf.fr) 97/10/02
       98/11/04 srio@esrf.fr adds Catch. Use of /Dir kw in Dialog_Pickfile().
       99/01/12 srio@esrf.fr fixed doc.
```

#XOP on-line help file: xplot.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/wutil/xplot.pro -----

============================ XPLOT ====================

XPLOT is a general package for creating X-Y plots that also allows for sophisticated data visualization, processing, manipulation and analysis. Some of the XPLOT features are:

1) Direct loading of data from multicolumn ASCII files. Multiple sets of data can be accessed from several files and merged together. Interactive action on data columns with the creation of new data from scratch or by manipulating existing data
2) Access to SPEC data files
3) Direct printing from Unix workstations and PCs, and creation of PostScript and encapsulated PostScript files
4) Linear and logarithmic X- and Y-axes. Apply and change symbols, line styles, colors, thickness, fonts etc.
5) Label, annotate, add legends, titles, etc. to the plots. Zoom, shift, switch columns, and over-plot data.
6) Save and restore plots and attributes in a XPLOT backup file.
7) Data analysis: extrema, moments, integrals, derivatives, CDFs, smoothing, user-defined operations, interactive Fourier filtering, interpolations, convolutions and correlations. It also includes several fitting routines: linear regression, polynomial fit, Gaussian fit and nonlinear fit (the gradient-expansion algorithm or the Powell method) with an on-line user-defined function.

XPLOT also includes some packages for specific data analysis. At present the XAID package for XAFS (X-ray Absorption Fine Structure) analysis is available. New applications and interfaces for data processing applied to different synchrotron techniques are under development, and they will be integrated in future releases.

On line help is available in most of the cases. A Web Xplot page and documentation can be found at:
http://www.esrf.fr/computing/scientific/xop/xplot

Overplotting with Xplot
==========

One of the most important features of Xplot is the capability to display multi-line graphs with data coming fro different origins. Data in Xplot is structured in the so-called sets.

A set is an array or matrix containing N points (or rows) and M columns.

Xplot stores the data in multiple sets, and each set may hold a different number of points or columns. Xplot allows multi-line plots, in which the data for each line is a couple of columns from a given set. Xplot options Calculations and File/Load Data File... allows to create new columns in defined sets and new sets from files or from operations between existing sets.

You can change the X and Y columns for the plot in the current set of data by just typing the column numbers in the bottom of the Xplot window. It is very important to enter <Enter> after modifying any text widget in Xplot. That permits Xplot to understand you have finished with the editing, and process the event.

If you want to do a plot with multiple lines, first load the data set with the first line. Then use the "Save Plot" button to store this set

as a "saved set". At this moment, the saved set is copied to the current set, and both will be displayed. Then, you can change columns of even load a new data set using File/Load menu and the new data set will be overplotted on the saved one. Repeat this process as many times as you want. Once a set is saved, the Xplot controls do do affect it. The window created by pressing the "Plot Mgr" (Plot manager) button permits to delete save sets, or to promote a saved set to the current set.

Xplot has been written by:

Manuel Sanchez del Rio
European Synchrotron Radiation Facility
BP 200
38043 Grenoble−Cedex 9
Email: srio@esrf.fr

========== USE OF XPLOT FROM THE IDL PROMPT ==========

NAME:
XPLOT
PURPOSE:
to plot and interactive manipulate data
CALLING SEQUENCE:
XPLOT [,indata] [,keywords]
OPTIONAL INPUT PARAMETERS:
indata can be one of the following:
1) filename: a string containing the file name to be plotted or an idl variable [fltarr(n_points,n_columns] with data. The file must be ascii data arranged in columns. Lines starting with characters [except . + −] are comments and not considered for the plot.
2) an idl variable containing the numerical data set (a fltarr(n_columns,n_points)
3) x,y two arrays with the abscissas and ordinate arrays.
4) h an IDL handler pointing to a set or to a number of sets.

KEYWORD PARAMETERS:
GROUP = The widget ID of the widget that calls Xplot. When this ID is specified, a death of the caller results in a death of Xplot.
WINDOW_SIZE = a 2−dim vector containing the width and height of the graphical window (in pixels).
XCOL = for multicolumn entries, the column number to be plotted in the X axis (default=1)
YCOL = for multicolumn entries, the column number to be plotted in the Y axis (default=last column)
WTITLE = title for the main window
TITLE = title for the plot
XTITLE = abscissas title. In the case that xtitle is set as XTITLE='−1', then xplot will place the text of COLTITLES corresponding to the plotted column.
YTITLE = ordinates title. In the case that ytitle is set as YTITLE='−1', then xplot will place the text of COLTITLES corresponding to the plotted column.
COLTITLES = string array with column labels.
LEGEND = A legend call to the LEGEND procedure by F K Knight (knight@ll.mit.edu)
STATE = a xplot state structure (only for internal use of Xplot (when creating clones))
PARENT = The wiggler id of the main Xplot window created. This is useful to pass this id as parent of other widgets that must die when the present XPlot window dies.
[XY]LOG = when set to 1, initializes [XY] logaritmic axis.
SPEC = input, initialize xplot with a SPEC file. Input may be a file name (string) or a spec handler (str). Example, IDL> xplor,spec='file.dat'
XRANGE=[xmin,xmax] range of the x variable for the plot
YRANGE=[ymin,ymax] y

OUTPUTS:
Open a widget utility and present a graphic.
COMMON BLOCKS:

SIDE EFFECTS:
If not active, starts Xmanager
RESTRICTIONS:
Unknown.

```
 PROCEDURE:
        Uses the PLOTFILE routine for producing the plot
 KNOWN BUGS:

        When starting xplot with coltitles keyword, the "clone"
          option does not work.
        [xy]title='-1' does not work properly with spec/mca data.

        Using Edit/Data and removing data causes xplot to
        crash when SPEC data is used or "-1" is used in titles.
        The automatic selection in Edit/Data does not work for
        data set in which the abscissas are reversed.

        The Save/Restore backup option is not very robust. It may
        give problems using complicated plots. It does not work with
        SPEC files. It may present incompatibilities between different
        xplot versions.

 MODIFICATION HISTORY:
by  Manuel Sanchez del Rio. ESRF. December 1993
        94-01-21 MSR improves the evaluate option
        94-02-02 MSR add style options in LIMITS menu
        94-02-18 MSR removes common blocks and allow
                multiple copies of the widget
        94-05-19 MSR fix a bug in the print buffer managment
                found by R. Dejus.
        94-06-27 MSR adds the /Calculations/correlation function
                option.
        94-11-17 MSR adds Tools/Xplot and Tools/IDL_command options
        95-02-11 MSR adds Calculations/Fitting option, check
                existence of input files.
        95-03-08 MSR: updating of fourierfilter: we pass now also
                the abscissas values.
        95-08-08 MSR: adds LEGEND keyword.

        95-09-14 MSR Releases Xplot version 2.0
        Nov 1995  version 2.1 major upgrades:
                - Integration and interfacing of spec_acces
                - COLTITLES keyword
                - Options Polynomial and Gaussian fit integrated
                in a single one.
                - new interface of non-linear fit.
        96-01-18 srio@esrf.fr changes xtext call by xedit from RJD.
        96-01-19 srio@esrf.fr adds options [xy]title='-1'
        96-01-22 srio@esrf.fr adds the possibility to edit column
                titles for SPEC files, and number the columns.
        96-04-12 srio@esrf.fr adds /xlog and /ylog kws. Change
                fieldlen in settitles.
        96-05-29 srio@esrf.fr xplot/title: when using spec files,
                the symbol #x (i.e. #S) is interpreted as its
                corresponding value in the spec scan header.
        96-07-09 srio@esrf.fr Adds SPEC keyword.
        96-08-13 srio@esrf.fr changes "'" by '"' in xplot_plot
        96-08-20 srio@esrf.fr makes the main window resizable,
                and removes the ZoomSel button (now automatic selection
                of zooming area by dragging the mouse with the left
                button down). Do not write intermediate files
                for view/showData. Introduce xhelp.
        96-12-04 srio@esrf.fr add "catch" in xplot_event to
                avoid crassing the application when there is an error.
        97-01-15 srio@esrf.fr complete the list of spec functions in
                xplot_compile().
        97-02-17 srio@esrf.fr debugging: log->lin change when saving,
                dynamic_resize of column widgets, correct cursor
                read-out when switching between Xplot windows. Add
                path to pickfile and uses xhelp for help.  Version 2.2
        97-06-27 srio@esrf.fr added View/Mesh option. version 2.2.
                Use copy_structure to restore backup file (assures
                compatibility between save files from different xplot
                versions).
```

97-09-07 srio@esrf.fr added non-interactive use of xplot.
Version 2.4
97-09-30 srio@esrf.fr substitutes read_ascii to rascii
97-10-27 srio@esrf.fr version 2.5, with lots of modifications:
New zoom rubberband code. Re-load file. Apply
button in many windows. Changed many calculations
windows (smooth, convolution, etc), non-linaer fit
with fixed parameters, new Plot Manager button
obsoleting the Set Current one, fixed many bugs
regarding zoom limits and resizing, etc, etc.
97-11-10 srio@esrf.fr adds Edit/Data... menu using xtable.
97-12-03 srio@esrf.fr adds xplot_cleardata() and fix
a bug with non-interactice use of plotmgr. V 2.5.1.
Adds xplot_setlimits().
98-02-18 srio@esrf.fr adds NOREFRESH keyword to
xplot_[setlimits,loadfile,changecol,exebuffer,
errorbars,addcol,plotmgr] routines.
Fix a bug (not displaying error bars in saved
sets.)
98-03-25 srio@esrf.fr small changes to allow starting
xplot when spec_access is not available.
98-04-07 srio@esrf.fr removed /no_copy kw in main
widget_draw definition (problems in w95).
98-09-18 srio@esrf.fr Avoid changing columns when reloading.
Improved SPEC window. Avoid changing columns
after column operations. Corrected bug in
displaying calculations,FWHM.../Max x.
Improved save/asciioption. Improved oper w columns.
Correct managment of ![x,y].style. Many other things.
Version 2.6.Beta1.
98-09-25 xplot_mesh and xplot_shift added
98-09-30 bug when selecting columns after adding cols fixed.
Use of psysvar when overplotting after fit.
Shortened "command" in xplot_plot
Other cosmetics.
98-09-30 reintroduced changes for PSD (done in revision 1.35
but lost). Version 2.6Beta3.
98-11-16 fixed a bug when applying oper w cols and the
coltitles kw is set. Shorts the number of
characters in the column pulldown menus.
Version 2.6Beta4.
98-11-20 fixed a bug when save/restore backup file.
Added "add to file" for spec files. Version 2.6Beta5.
99-01-08 substituted cw_clr_index by cw_clr_index1 to allow
entering the index by simple typing.

99-01-13 Removed calls to xaid.
99-03-12 Added non-modal window for setting limits. Help
menu updated. Pemoved xplot_compile. Added
option to Wrile/Load qattributes from file.
Aded hardware and TT fonts. Version 2.7B1
00-03-21 Improved Calculation|Interpolation/Spline option
01-01-22 Improving Edit|Cut
01-01-24 Allows printing a zoomed image. Improves
operations with sets...
Fixed bugs in Edit|Columns (with columns labels and
SPEC)
02-03-08 srio@esrf.fr adds AutoReLoadFile option. The autoreload
if the file has been modified works only for idl >= 5.5
02-03-13 srio@esrf.fr changed PolyFitW by Poly_Fit
02-05-27 srio@esrf.fr Bug fixed: Added /SORT kw to
Int_Tabulated calculations (before it returned wrong
values when the array was sorted in descendent order)
02-06-20 srio@esrf.fr manages the spec keywords with
more than one character in the xplot title label.

================ NON-INTERACTIVE MANIPULATION OF XPLOT ==========

Since Xplot version 2.4, the Xplot internals are being modified
to allow also non-interactive manipulation of Xplot.
This is very useful when using Xplot from other widget applications
and one wants to prepare sophisticated plots with options not
availables as keywords in the main Xplot call. Typical examples
are to overplot several plots, to add commands in the EXEbuffer,
or to display error bars.
The access is done by a set of routines with general syntaxis:

xplot_<name>, parent [,other_inputs, keywords]

where <name> indicates the action to be performed (i.e. loadfile,
quit, etc.), parent is the widget id of the manin Xplot window to
be manipulated and the other information is passed using the
other inputs and keywords.

EXAPLE:

```
        ; you can execute these commands as an example
        tmp = fltarr(5,100)
        tmp(0,*) = findgen(100)
        tmp(1,*) = tmp(0,*)^2     ; first curve
        tmp(2,*) = tmp(0,*)^2+100 ; second curve
        tmp(3,*) = tmp(0,*)^2-500 ; bottom of error bars
        tmp(4,*) = tmp(0,*)^2+500 ; top of error bars
        xplot,parent=p,/no_block  ; starts xplot, retrieved parent id
        xplot_loadfile,p,tmp      ; load the data in xplot
        xplot_changecol,p,ycol=3  ; set Y as column 3
        xplot_controls_action,p,linestyle=1 ; set dotted line
        xplot_savecurrent,p       ; save this plot
        xplot_changecol,p,ycol=2  ; overplot column 2
        xplot_controls_action,p,linestyle='0' ; overplotted line to soli
d
        xplot_errorbars,p,4,5     ; plot error bars
        xplot_exebuffer,p,setbuffer=$ ; add an annotation
                "xyouts,.2,.7,'Example of non-interactive label',/norm"
```

Available routines are:

```
        xplot_quit
        xplot_cleardata
        xplot_setlimits
        xplot_loadfile
        xplot_savecurrent
        xplot_changecol
        xplot_exebuffer
        xplot_errorbars
        xplot_addcol
        xplot_plotmgr
        xplot_saveascii
        xplot_mesh
        xplot_shift
        xplot_controls_action
        xplot_reloadfile
        xplot_autoreloadfile
```

The routines help id listed below.

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_QUIT
        PURPOSE: Quits the Xplot window and destroy the internal handlers.
        CALLING SEQUENCE: XPLOT_QUIT,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)
        MODIFICATION HISTORY:
                97-09-11 srio@esrf.fr initial version from xplot code
```

This routine is part of the xplot package. It is used internally by xplot, but it also permits to manipulate non-interactively the xplot window. Only the last feature is documented here.

NAME: XPLOT_CLEARDATA
PURPOSE: clears graphs in xplot
CALLING SEQUENCE: XPLOT_CLEARDATA,parent
INPUTS:
KEYWORD PARAMETERS:
        CONFIRM = When set, display a confirmation window.
MODIFICATION HISTORY:
        97-12-03 srio@esrf.fr initial version from xplot code

```
This routine is part of the xplot package. It is used internally
by xplot, but it also permits to manipulate non-interactively
the xplot window. Only the last feature is documented here.

NAME: XPLOT_SETLIMITS
PURPOSE: Sets the xrange and/or yrange to xplot.
CALLING SEQUENCE: XPLOT_SETLIMITS,parent
INPUTS:
        PARENT the widget id of the main Xplot window to
        It has to be retrieved when the main window is created:
        PARENT = 0 ; initializes the variable
        Xplot,...,PARENT=parent ;stores widget id in parent (named
        variable)

KEYWORD PARAMETERS:
        XRANGE = [xmin,xmax] The extrema in X
        YRANGE = [ymin,ymax] The extrema in Y
        XSTYLE = The XSTYLE Graphic Keyword (see IDL doc)
        YSTYLE = The YSTYLE Graphic Keyword (see IDL doc)
        NOREFRESH set this keyword to avoid refreshing the graph
                after the loading process. Useful when loading
                many curves.

MODIFICATION HISTORY:
        97-12-03 srio@esrf.fr initial version from xplot code.
        99-03-10 srio@esrf.fr adds xplot_setlimits_interactive
                for non-modal interactie change of limits.
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_LOADFILE
        PURPOSE: load a file or variable in xplot
        CALLING SEQUENCE: XPLOT_LOADFILE,parent [,input,spec=spec]
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

                INPUT  it can either be:
                   1) a string with the ASCII file name
                   2) an idl variable with a multi-column set (i.e.  fltarr(2,10
0) )
        KEYWORD PARAMETERS:
                SPEC set this keyword to a SPEC file name. In this case the
                file is loaded and interpreted as SPEC file. IN this case,
                "INPUT" is not used.
                PLOTNAME set this keyword to a string that identifies the
                        plot (to be used by plotmgr).
                NOREFRESH set this keyword to avoid refreshing the graph
                        after the loading process. Useful when loading
                        many curves.
                SCANID When using SPEC input, set this keyword to the
                        scan id to be loaded (e.g., 'CURRENT').  Default='LAST'
                WTTILE Title for the main window bar

        MODIFICATION HISTORY:
                97-09-11 srio@esrf.fr initial version from xplot code
                97-12-03 srio@esrf.fr adds plotname keyword.
                98-02-17 srio@esrf.fr adds norefresh keyword. Xplot v 2.5.2
                01-02-23 srio@esrf.fr adds wTitle keyword.
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_SAVECURRENT
        PURPOSE: to save the current displayed plot in xplot (same
                effect as pressing the "Save Current" button on the xplot
                window)
        CALLING SEQUENCE: XPLOT_SAVECURRENT,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        MODIFICATION HISTORY:
                97-09-11 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_CHANGECOL
        PURPOSE: to change the X or Y displayed column in xplot
                It works aso with SPEC files, including MCA. In the last
                case the (X) column for Channels is ncol+1 and for Energy
                is ncol+2, being ncol the number of channels.
        CALLING SEQUENCE: XPLOT_CHANGECOL,parent ,XCOL=xcol, YCOL=ycol
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS [USE AT LEAST ONE]:
                XCOL The column index for X (starting from col 1, not 0)
                YCOL The column index for Y (starting from col 1, not 0)
                NOREFRESH set this keyword to avoid refreshing the graph
                        after the loading process. Useful when loading
                        many curves.

        MODIFICATION HISTORY:
                97-09-11 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_EXEBUFFER
        PURPOSE: to set a buffer or to add commands to the buffer
                The EXEbuffer is a set of IDL commands that are executed
                after the plot. It is used to make labels, annotations, etc.
        CALLING SEQUENCE: XPLOT_EXEBUFFER,parent, ADDBUFFER=addbuffer, $
                SETBUFFER=setbuffer
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS [MUST USE ONLY ONE (MUTUALLY EXCLUSIVE)]:
                ADDBUFFER A string array with the commands to be added to the bu
ffer

                SETBUFFER A string array with the commands to be set to the buff
er.
                        If the buffer contained commands, they are deleted befor
e.
                NOREFRESH set this keyword to avoid refreshing the graph
                        after the loading process. Useful when loading
                        many curves.

        MODIFICATION HISTORY:
                97-09-11 srio@esrf.fr initial version from xplot code
```

```
This routine is part of the xplot package. It is used internally
by xplot, but it also permits to manipulate non-interactively
the xplot window. Only the last feature is documented here.

NAME: XPLOT_ERRORBARS
PURPOSE: create error bars on a given plot
CALLING SEQUENCE: XPLOT_ERRORBARS,parent, col1, col2
INPUTS:
        PARENT the widget id of the main Xplot window to
        It has to be retrieved when the main window is created:
        PARENT = 0 ; initializes the variable
        Xplot,...,PARENT=parent ;stores widget id in parent (named
                variable)
        COL1 the column containing the bottom limit of the error bars
        COL2 the column containing the upper limit of the error bars
        NOREFRESH set this keyword to avoid refreshing the graph
                after the loading process. Useful when loading
                many curves.
MODIFICATION HISTORY:
        97-09-11 srio@esrf.fr initial version from xplot code
```

This routine is part of the xplot package. It is used internally by xplot, but it also permits to manipulate non-interactively the xplot window. Only the last feature is documented here.

NAME: XPLOT_ADDCOL
PURPOSE: load a numerical array and include it as new column in Xplot.
CALLING SEQUENCE: XPLOT_ADDCOL,parent,input
INPUTS:
PARENT the widget id of the main Xplot window to
It has to be retrieved when the main window is created:
PARENT = 0 ; initializes the variable
Xplot,...,PARENT=parent ;stores widget id in parent (named variable)

INPUT an array with the new column.

KEYWORD PARAMETERS:

MODIFICATION HISTORY:
97-10-21 srio@esrf.fr initial version slightly modifying the old xplot_addcol.

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_PLOTMGR
        PURPOSE: manage the saved set (delete or move to current).
        CALLING SEQUENCE: XPLOT_PLOTMGR,parent [,selected ]
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

                SELECTED = the saved set number (starting from 1) to be
                edited (moved or deleted).
        KEYWORD PARAMETERS
                [THE FOLLOWING ONES ARE EXCLUSIVE. AT LEAST ONE IS MANDATORY]:
                DELETE_SEL will delete the selected saved set.
                DELETE_ALL will delete all the saved sets.
                MOVE will move the selected saved set to the current set.
                [GENERAL KWYWORDS]:
                NOREFRESH set this keyword to avoid refreshing the graph
                        after the loading process. Useful when loading
                        many curves.

        MODIFICATION HISTORY:
                97-10-24 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_SAVEASCII
        PURPOSE: save to an ascii file the current set
        CALLING SEQUENCE: XPLOT_SAVEASCII,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        MODIFICATION HISTORY:
                98-08-25 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_MESH
        PURPOSE: displays mesh data
        CALLING SEQUENCE: XPLOT_MESH,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS [USE AT LEAST ONE]:
                FLAG 0 displays data in usual mode (no-mesh)
                     1 displays data in mesh mode
                KIND 0 show mesh plot with lines
                     1 shadow mesh plot with a surface
                     2 shadow mesh plot with contour curves
                     3 shadow mesh plot with a shaded surface
                POINTS set this keyword to the number of points of each individu
al
                        curve in the total data
                COL set this keyword to a column indicating containing the index

                        to recognise individual curves
                        (the COL and POINTS keyword are exclusive. If both are s
et,
                        only COL is used.)
                KEYWORDS string with extra keywords to be passed to the graphica
l
                        routines.

        MODIFICATION HISTORY:
                98-09-24 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_SHIFT
        PURPOSE: adds a horizontal and vertical shift to the current set
        CALLING SEQUENCE: XPLOT_SHIFT,parent [,openwindow,set_value=set_value]
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS:
                OPENWINDOW when set, opens a widget window for interactive
                manipulation
                SET_VALUE a 2-element array [h,v] with the shift to be applied
                to the horizontal (h) and vertical (v) axes.

        MODIFICATION HISTORY:
                98-09-17 srio@esrf.fr initial version.
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_CONTROLS_ACTION
        PURPOSE: to change plot attributes in XPlot (i.e. Log plots,
                symbols, thicknesses, colors, etc). In other words,
                permits the non-interactive manipulations of all the
                controls under the "Show Controls" button.
                If the "Show Controls" window is opened, it also updates it.

        CALLING SEQUENCE: XPLOT_CONTROLS_ACTION,parent [, keywords]
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS [USE AT LEAST ONE]:
                Note that some keyword values are assigned to zero. For
                setting them use KEYWORD='0', because KEYWORD=0 means not
                setting the keyword. For non-zero values, both KEYWORD='n'
                and KEYWORD=n are, in general, accepted.

                PSYMSIGN set plot to concected (PSYMSIGN='0') or disconnected
                        (PSYMSIGN='1') line.  This keyword does not make any
                        effect if PSYMBOL='0'
                PSYMBOL set symbol:
                        '0' line
                        1 +
                        2 *
                        3 Period
                        4 Diamond
                        5 Triangle
                        6 Square
                        7: X
                        8: User-defined
                        9: undefined
                        10: histogram
                LINESTYLE define the line style:
                        '0' Solid
                        1 Dotted
                        2 Dashed
                        3 Dash-Dot
                        4 -...-...
                        5 Long dash
                KIND log or lin plots in X/Y:
                        '0' lin/lin
                        1   lin/log
                        2   log/lin
                        3   log/log
                TICKLEN internal/external ticks or grid
                        '0' internal
                        1   external
                        2   grid
                THICK <float> the line thickness
                CHARSIZE <float> the character size
                CLR_BACK <integer> the background color
                CLR_AXIS <integer> the axis color
                CLR_LINES <integer> the lines color
                CLR_RESET set this keyword to reset the original background,
                        axis and lines colors.
                CLR_DEFAULT set this keyword to set the color table to the
                        default one (B&W + Tek_Color)
                FONT selects a font
                       Index 0 -> 3:  Simplex Roman
                       Index 1 -> 4:  Simplex Greek
```

```
                Index 2 -> 5:  Duplex Roman
                Index 3 -> 6:  Complex Roman
                Index 4 -> 7:  Complex Greek
                Index 5 -> 8:  Complex Italic
                Index 6 -> 9:  Math and Special
                Index 7 -> 10: Special
                Index 8 -> 11: Gothic English
                Index 9 -> 12: Simplex Script
                Index 10 -> 13: Complex Script
                Index 11 -> 14: Gothic Italian
                Index 12 -> 15: Gothic German
                Index 13 -> 16: Cyrillic
                Index 14 -> 17: Triplex Roman
                Index 16 -> 18: Triplex Italic
                Index 16 -> hardware font
                Index 17,18,... -> TT Fonts (as returned by
                        TT_Font_manager)
        NOREFRESH set this keyword to avoid refreshing the graph
                after the loading process. Useful when loading
                many curves.

MODIFICATION HISTORY:
        97-09-11 srio@esrf.fr initial version from xplot code
        99-03-12 srio@esrf.fr adds Hardware and TT fonts
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_RELOADFILE
        PURPOSE: re-load a file or variable in xplot
        CALLING SEQUENCE: XPLOT_RELOADFILE,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS:

        MODIFICATION HISTORY:
                2002-03-06 srio@esrf.fr initial version from xplot code
```

```
        This routine is part of the xplot package. It is used internally
        by xplot, but it also permits to manipulate non-interactively
        the xplot window. Only the last feature is documented here.

        NAME: XPLOT_AUTORELOADFILE
        PURPOSE: re-load a file or variable in xplot
        CALLING SEQUENCE: XPLOT_RELOADFILE,parent
        INPUTS:
                PARENT the widget id of the main Xplot window to
                It has to be retrieved when the main window is created:
                PARENT = 0 ; initializes the variable
                Xplot,...,PARENT=parent ;stores widget id in parent (named varia
ble)

        KEYWORD PARAMETERS:
                Action = One of the following strigns (case sensitive):
                        'Preferences...' Pops-up the preferences window
                        'Start' Start timer (autoreload) mode
                        'Stop' Stop autoreload mode
                SET_CHECK: Flag for controlling the updating (autoreload):
                        0: ALways reload file
                        1: Reload file if it has been modified
                SET_TIMER: Time [sec] waited between realods

        EXAMPLE:

                xplot,Parent=p,/No_Block
                xplot_Loadfile,p,'xplot.dat'
                xplot_AutoReLoadFile,p,Set_timer=1.0
                xplot_AutoReLoadFile,p,Action='Start'
                xplot_AutoReLoadFile,p,Action='Stop'

        MODIFICATION HISTORY:
                2002-03-08 srio@esrf.fr initial version
```

#XOP on-line help file: xpower.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/optics/xpower.pro ---
--

============================ Xpower ==================================

Xpower is a widget based graphical interface to calculate the transmission in terms of flux or spectral power energy as a function pf photon energy for a set of up to five attenuators and mirrors.

It uses the DABAX files to get reflectivities and transmissions.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Xpower input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main XPower window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, XPower starts running.

If you whish to calculate values for a single energy point instead of an array of energy points [default], set the energy minimum equal to the energy maximum. In this case, the results will be presented in a common text window for all the three options in the "Show" menu.
Set Defaults: Sets the default parameters.

Show: Produces a graphic of the results (Local properties, cumulated properties) and shows text parameters. In the case that a single energy point is calculated (by setting the minimum energy equal to the maximum energy), the three menu entries will display the same text parameters.

Help: Shows the xpower help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xpower_par.txt

This screen holds the inpout parameters for XPOWER

It consists of the following entries:

f1f2 datasets \
> The dabax datasets with f1f2 and Mu for
Mu datasets / reflectivity and transmission (respectively).

Source: Select one of the following possibilities:
1) Normalized to 1 (standard E grid): The source is normalized to 1 and the energy array consist in 500 points in the [1,100] keV interval.
2) Normalized to 1 (E grid from keyboard): The source is normalized to 1 and the energy starting point, ending point and number of points are entered from the keyboard (next entries). The number og points must be greater than one. For calculating a single energy point, set the starting and the ending value to the same value.
3) From external file: The energy [in eV] and source arrays are thetwo first columns of the given file. In the case that the file does not exist, it asks for a new one. Therefore, by entering any string (e.g. '?'), a browser to select the file will be launched.
4) xop/source Flux (file SRCOMPE) the source fnd energy arrays are read from the SRCOMPE file, which is usually produced by a xop/source calculation.
5) xop/source Power (file SRCOMPW) the source fnd energy arrays are read from the SRCOMPW file, which is usually produced by a xop/source calculation.

If selected source is case 2, then entry the start, end and number of E points.
If selected source is 3, entry the file name.

Number of elements: The number of optical elements for calculations (from 1 to 5).
For each optical elements a line of entry boxes appear with the following meaning:

xx oe formula: The optical element formula. This may be an element or compound formula (i.e. Si, H2O, etc.), a mixture formula (i.e. H2O(0.99)Cl2(0.01)), or a material name as defined in the DABAX file Compounds.dat The list of the material defined in the installed Compounds.dat file is listed below. It is possible to type a question mark (?). In this case the program will present a list with all the available compounds in the Compounds.dat file, and the user must select one. This avoids typos in typing the compound names.
Filter/Mirror (select the appropiate entry).
In the Flter case entry the filter thickness [mm]
In the Mirror case entry the grazing angle [mrad] and the surface roughness rms [Angstroms]
Density: The density value in g/cm^3. It accepts the ? entry. In such a case it takes:
- For elements, the value returned by AtomicConstants()
- For materials from the Compounds.dat file, the value stored in that file.
- Takes 1.0 as defaults in the other cases.

==========

The allowed compound names [from file Compounds.dat] are listed below.
(Case sensitive!. Do not add blanks at the beginning or end of the name.
Remember that this list appears interactively when a "?" is typed.)

#XOP on-line help file: xtc.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xtc.pro -----
================================== Xtc ==================================

Xtc is an widget based graphical user interface to calculate on-axis brilliance tuning curves for an ideal undulator insertion device using the Bessel function approximation (regular planar device or helical device). The calculation is performed by the program TC ("tuning curves") which is executed from the XTC interface. The effects of the particle beam emittance and beam energy spread are taken into account.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
Xtc input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
TC file: This option allows to load/write the current parameter and result files for further calculations. The used file formats are those used by TC. Therefore, they can be used to run TC without the interface or to import TC files created outside the XTC application.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main XTC window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, TC starts running.
Set Defaults: Sets the default parameters.

Show: Display results
Plot ...: Plots the different TC results.
View Results: Displays the TC result file, tc.out, in a scrollable window. The file may be printed from this window.

Help: Shows the TC help and the XTC help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

LAST MODIFICATION: msr/rjd/00-07-12

#XOP on-line help file: xtopo.txt

----- file created by makedoc on: Thu Feb 6 15:33:46 2003

#XOP on-line help file: xtube_w.txt

================================ xtube_w ================================

xtube_w is an widget based graphical interface to calculate the spectum of a Tungsten X-ray tube.

It uses a routine routine to generates spectra (photons/mm**2 per keV) for one mAs and the output is calibrated to the output of a constant potential generator in our laboratory (a Toshiba Model 2050 x-ray generator with a "Rotanode" x-ray tube with housing model DRX-573HD-S and insert model DR-5735H).
These spectra were calibrated to output (mR/mAs) values and HVL values that were measured down the central axis of the x-ray beam. The output data are given in the manuscript:
"An accurate method for computer- generating tunsten anode x-ray spectra from 30 to 140 kV", JM Boone and JA Seibert, Medical Physics 24(11) pp.1661-1670, November 1997.

The program interfaced by XTubeW has been downloaded from:
ftp://ftp.aip.org/epaps/medical-phys/E-MPHYA-24-1661

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Xtube_W input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
  Write Files for XOP/Optics: Saves the current undulator spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files to be used for the other XOP application from Optics menu.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main Xtube_w window.
Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, xtube_w starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Plot Results: Plots the xtube_w rsult: flux per sec per 1 keV bandwidth and per mm^2 collected at 1 m from the target.

Help: Shows the xtube_w help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations using the xtube_w aplication

should also cite:

J.M. Boone and J.A. Seibert "An accurate method for computer−generating tunsten anode x−ray spectra from 30 to 140 kV", Medical Physics 24(11) pp.1661−1670, 1997.

LAST MODIFICATION: msr/msr/03−01−08

#XOP on-line help file: xtubes.txt

========== xtubes ==========

xtubes is an widget based graphical interface to calculate the spectum of an X-ray tube with Mo, Rh or W target in the energy range 18-40 keV.

It uses the method descibed in the manuscript:
"Molybdenum, rhodium, and tungsten anode spectral models using interpolating polynomials with application to mammography"
J.M. Boone T.H. Fewell and R. J. Jennings
Medical Physics 24(12) pp. 1863-1874, 1997.

The program interfaced by XTubeW has been downloaded from:
ftp://ftp.aip.org/epaps/medical-phys/E-MPHYA-24-1863

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  xtubes input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
  Write Files for XOP/Optics: Saves the current undulator spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files to be used for the other XOP application from Optics menu.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main xtubes window. Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, xtubes starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Plot Results: Plots the xtubes results (see note on units).

Help: Shows the xtubes help (this text).

NOTE ON RESULT UNITS:
  The units of the fluence in the results are not very clear in the Boone's paper. This has creates some problems for users, and originated a discussion between Sutter (sutter@ntmail.desy.de) and Boone. You can find below a short version of the discussion:

  In the paper for the W (only) [XOP program xtube_w] Boone's paper clearly states that the flux per sec per 1keV bandwidth and per mm2 collected at 1m from the target. The result looks very reasonable, and I (srio@esrf.fr) have checked one result against the example in the doc of "Catalogue of diagnostic x-ray spectra and other data", Cranley et al., Report 78, The Institute of Physics and Engineering in Medicine, with quite reasonable agreement. However, in the paper on Mo, W and Rh [code Xtubes] the units are not clearly stated. Moreover, both programs produced different results for W @ > 41 keV (one case that can be calculated with both codes).

  I (sutter@ntmail.desy.de) have had several interesting exchanges with Dr. Boone.
    The units: The paper on Mo, W, and Rh states that the spectra

collected on these tubes were binned into 500 eV intervals. (See Fig. 2 for an example of these spectra for the Mo anode.) In addition, the caption of Fig. 2 states that all the spectra were normalized to a constant value of mA x sec, but does not reveal what this value was. When I asked Boone about this, he said that his reason for not revealing it was the following:
"You are correct, I intentionally did not "reveal" the absolute output efficiency of the x−ray sources because x−ray tubes are so variable − the calibration of the mA (and the time) is often imperfect (and hence the mR/mAs term would be in error) and the amount of inherent x−ray tube filtration (we deal with tubes in the clinical environment, which have collimators and other structures over the x−ray tube port which make it difficult and impractical to visually check exactly what filters are in the beam. Thus, the total inherent (and added) filtration is often not known.)"
When I pressed him for at least an approximate value for the normalizing constant, he stated that it was 1 mA x sec. However, the above warning about the variability of X−ray tubes should be kept in mind.

In short, the units for the fluence, strictly speaking, should be: photons/mm2/500 eV/(mA.s).

One final note: Boone stated in another message to me that the fluence from a point source drops off with the inverse square law. This indicates that the area unit (mm2) in the fluence refers to the number of photons per unit surface area on a sphere of given radius centered on the anode, rather than to the number of photons produced per unit illuminated area on the anode.

Another quantity that isn't given with certainty in Boone's first paper is the distance between the Mo, Rh, and W tubes and the detector. When I asked Boone for this quantity, he said it was "probably 50 cm," this being a common distance for mammography measurements.
The measurements for the W tube in Boone's second paper, corresponding to the XOP program "xtubes_w", however, are clearly stated to have been made at 1 m from the tube.
Perhaps this explains the discrepancy between the results from the two calculation routines xtube_w and Xtubes . Does this make sense? (The fact that 500−eV bins are used in the first paper, while the fluence in the second is given per 1 keV bandwidth, will also influence the results.)

Added srio@esrf.fr: Following this arguments, in order to transform the units of xtubes (fluence @0.5m with 0.5keV bandwidth) into xtube_w units (fluence @1m with 1keV bandwidth) one should multiply by (0.5/1.0)^2 * 2 = 1/2 (in other words, at 1m we have 1/4 times the flux of at 0.5m multiplied again by 2 because we use the double of bandwidth). However, a strage factor of about 1000 is found:

W @ 41 kV

Photon_Energy[keV]	Fluence[xtube_w]	Fluence[xtubes]
25	1.24e4	1.23e7
35	7.02e3	4.39e6

I have no explanation for this discrepancy.

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340−345, 1998.

In addition, published calculations using the xtubes aplication should also cite:

J.M. Boone T.H. Fewell and R. J. Jennings "Molybdenum, rhodium, and tungsten anode spectral models using interpolating polynomials with application to mammography"
Medical Physics 24(12) pp. 1863–1874, 1997.

LAST MODIFICATION: msr/msr/99–03–16

#XOP on-line help file: xtubes_par.txt

Description of the input parameters for XTUBES:
==========

TARGET ELEMENT: Select one: Mo, Rh or W
VOLTAGE: Anode voltage in kiloVolts in the 18-42 interval.

#XOP on-line help file: xurgent.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xurgent.pro ----

========== Xurgent ==========

Xurgent is an widget based graphical interface to calculate
spectra of an undulator insertion devices.

It interfaces the program URGENT written by R.P.Walker and B.Diviacco
(see Help/Urgent)

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Xurgent input parameters: This option allows to save the current
              parameters to a file for later loading. It also allows
              to save the current parameters as defaults for being
              used when the application is initialized. In the last
              case, the file is named "application".xop (where
              "application " is the name of the current XOP
              application) and is written in the directory pointed
              by the XOP_DEFAULTS_DIR environment variable (which
              must be set). The parameter file is ASCII and can be
              read and edited with care.
  Urgent file: This option allows to load/write the current parameter
              and result files for further calculations. The used file
              formats are those used by URGENT. Therefore, they
              can be used to run URGENT without the interface or to
              import URGENT files created outside the XUrgent application.
  Write Files for XOP/Optics: Saves the current undulator
              spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files
              to be used for the other XOP application from Optics
              menu.
Quit: to exit from the program

Set_Parameters:
K(gap) Tool: This tool permits to calculate the deflection
              parameter K as a function of the magnet gap.
Set Parameters: to define the parameters for the calculation.
              The same result is obtained pressing the "Set Parameters"
              button in the main XUrgent window.
             Please refer to the information under the HELP
              button for a complete description of the parameters. After
              pressing the ACCEPT button, URGENT starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Plot Results: Plots the URGENT results.
  Show Numerical Results: Displays the URGENT result file.

Help: Shows the URGENT help and the XURGENT help (this text).

CREDITS:
       Published calculations made with XOP should refer:

         M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
         SPIE proceedings vol. 3448, pp.340-345, 1998.

       In addition, published calculations using the URGENT aplication
       should also cite:

R.P.Walker and B.Diviacco, "Urgent− A computer program for
calculating undulator radiation spectral, angular, polarization,
and power density properties.
Rev. Sci. Instrum. 63(1), pp. 392−395, 1992.

LAST MODIFICATION: msr/msr/00−06−14

#XOP on-line help file: xus.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xus.pro -----
============================== Xus ====================================

   Xus is an widget based graphical user interface to calculate
   spectral properties of ideal undulator insertion devices.

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    Xus input parameters: This option allows to save the current
                parameters to a file for later loading. It also allows
                to save the current parameters as defaults for being
                used when the application is initialized. In the last
                case, the file is named "application".xop (where
                "application " is the name of the current XOP
                application) and is written in the directory pointed
                by the XOP_DEFAULTS_DIR environment variable (which
                must be set). The parameter file is ASCII and can be
                read and edited with care.
    US file: This option allows to load/write the current parameter
                and result files for further calculations. The used file
                formats are those used by US. Therefore, they
                can be used to run US without the interface or to
                import US files created outside the XUS application.
    Write Files for XOP/Optics: Saves the current undulator
                spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files
                to be used for the other XOP application from Optics
                menu.
  Quit: to exit from the program

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                The same result is obtained pressing the "Set Parameters"
                button in the main XUS window.
                After pressing the ACCEPT button, US starts running.
  Set Defaults: Sets the default parameters.

  Show: Display results
    Plot ...: Plots the US results.
    View Results: Displays the US result file.

  Help: Shows the US help and the XUS help (this text).

 COPYRIGHT:
        XUS belongs to XOP package and it is distributed within XOP.
        PLEASE REFER TO THE XOP COPYRIGHT NOTICE BEFORE USING IT.

 CREDITS:
        Published calculations made with XOP should refer:

          M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
          SPIE proceedings vol. 3448, pp.340-345, 1998.

        In addition, published calculations using the US aplication
        may also cite:

          P. Ilinski, R.J. Dejus, E. Gluskun and T. I. Morrison
          SPIE proceedings vol. 2856, pp.15-25, 1996.

  KNOWN BUGS:
       When a us calculation producing 3D results is run, the Show/Plot 2D
        menu gives wrong results (MSR 98-12-04).

LAST MODIFICATION: rjd/msr/00-07-12

#XOP on-line help file: xwiggler.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:17 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xwiggler.pro -----

============================ Xwiggler ==================================

Xwiggler is a widget based graphical interface to calculate
the spectrum of a Wiggler Synchrotron Radiation source.

The Flux and Spectral Power values calculated with XWiggler
correspond to the integration in FULL vertical and horizontal
emission angles.

XWiggler calculations are done using the IDL program wiggler_spectrum.
This program is an IDL version of the Fortran program with the same
name available in the SHADOW ray-tracing package.

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  XWiggler input parameters: This option allows to save the current
              parameters to a file for later loading. It also allows
              to save the current parameters as defaults for being
              used when the application is initialized. In the last
              case, the file is named "application".xop (where
              "application " is the name of the current XOP
              application) and is written in the directory pointed
              by the XOP_DEFAULTS_DIR environment variable (which
              must be set). The parameter file is ASCII and can be
              read and edited with care.
  Write Files for XOP/Optics: Saves the current undulator
              spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files
              to be used for the other XOP application from Optics
              menu.
Quit: to exit from the program

Set_Parameters:
K(gap) Tool: This tool permits to calculate the deflection
              parameter K as a function of the magnet gap.
Set Parameters: to define the parameters for the calculation.
              The same result is obtained pressing the "Set Parameters"
              button in the main XWiggler window.
             Please refer to the information under the HELP
              button for a complete description of the parameters. After
              pressing the ACCEPT button, wiggler_spectrum starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Spectra: Plots the calculated wiggler spectra.
  Trajectories: Plots the calculated electron trajectories (individual paths
                      and 3D view)
  Parameters: Show the input parameters and some calculated values.

Help: Shows the XWiggler help (this text).

CREDITS:
       Published calculations made with XOP should refer:

         M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments"
         SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations using the XWIGGLER aplication could also cite:

C. Welnak, G.J. Chen and F. Cerrina, "SHADOW: a synchrotron radiation X-ray Optics simulation tool",
Nucl. Instr. and Meth. in Phys. Res. A347 91994) 344
or
SHADOW WEB Page: http://www.xraylith.wisc.edu/shadow/shadow.html

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xwiggler_par.txt

Description of the input parameters for BM:
==========

MAGNETIC FIELD three posibilities:
  Sinusoidal or standard wiggler
  Asymmetric wiggler with magnetic field profile (for a single priod)
    from a two columns file (y[meters], B[Tesla])
    An example of this option can be found in the files ex3_b.dat
        in the $XOP_HOME/examples directory.
  Asymmetric wiggler with magnetic field calculated in function of a
    supplied file containing the harmonic expansion of the magnetic field
    profile. The file contains two columns: (# of harmonic, Bmax [T])
    An example of this option can be found in the files ex3_b.dat
    in the $XOP_HOME/examples directory.
NUMBER OF PERIODS of the Wiggler
WIGGLER PERIOD in meters
K VALUE
BEAM ENERGY of the electrons in GeV
MINIMUM PHOTON ENERGY for the calculation in eV
MAXIMUM PHOTON ENERGY for the calculation in eV
NUMBER OF ENERGY POINTS
ENERGY POINT SPACING: Sel linear of logatithmic for the corresponding
        energy point spacing
NUMBER OF TRAJECTORY POINTS PER PERIOD of electron trajectory
ELECTRON BEAM INTENSITY in mA
EXTERNAL FILE with Magnetic field profile or Harmonic expansion. (Case of
  asymmetric wiggler). Type ? for starting a file browser to get it.

#XOP on-line help file: xxcom.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:18 2003
----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/optics/xxcom.pro ----
-

============================ Xxcom ====================================

Xxcom is a widget based graphical interface to calculate and display photon cross sections.

It interfaces XCOM, a computer program and data base to calculate photon cross sections for scattering, photoelectric absorption and pair production, as well as attenuation coefficients, in any element, compound or mixture, at energies from 1keV to 100GeV.

The XCOM program has been written by M.J. Berger and J.H. Hubbell at NIST (see Help/Xcom).

DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

File:
  Xxcom input parameters: This option allows to save the current parameters to a file for later loading. It also allows to save the current parameters as defaults for being used when the application is initialized. In the last case, the file is named "application".xop (where "application " is the name of the current XOP application) and is written in the directory pointed by the XOP_DEFAULTS_DIR environment variable (which must be set). The parameter file is ASCII and can be read and edited with care.
Quit: to exit from the program

Set_Parameters:
Set Parameters: to define the parameters for the calculation. The same result is obtained pressing the "Set Parameters" button in the main Xxcom window. Please refer to the information under the HELP button for a complete description of the parameters. After pressing the ACCEPT button, xcom starts running.
Set Defaults: Sets the default parameters.

Show: Display results
  Plot Data: Shows the output data with the XPLOT facility. It is possible to switch between the output quantities and to do a large number of operations and display presentations by using the XPLOT controls
  Numerical Data: Displays the output file.

Help: Shows the xcom help and xxcom help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations using the xcom aplication should also cite:
XCOM: Photon Cross Sections on a Personal Computer
M. J. Berger and J. H. Hubbell, Center for Radiation Research, National Bureau of Standards, Gaithersburg, MD 20899

LAST MODIFICATION: msr/msr/99-03-16

#XOP on-line help file: xxcom_par.txt

Description of xxcom input parameters:
==========

NAME: A title.
SUBSTANCE: Element, compound or mixture.

DESCRIPTION: Give the description formula for your substance. In the case SUBSTANCE=Element (Atomic Number) enter a integer with the atomic number. For SUBSTANCE= Element (Symbol) just enter the chemical symbol. For Compounds enter the formula (i.e H2O for water) and for a mixture enter the formulas of its components separated by ":".

FRACTION: Only available when SUBSTANCE=Mixture. Enter here the fraction of the total weight of each different constituents separated by ":"

GRID:
Standard (Log scale in the interval 1keV 100GeV)
Standard+points: standard + user defined points.
Points only: Only user-defined points

GRID POINTS: If GRID=Standard+points or Points only then the input energy values [in MeV] can either be entered from a file or from the keyboard.

GRID POINTS/FILE: If GRID POINTS=From keyboard, the energy values separated by ":", else the file name.

OUTPUT QUANTITIES: If SUBSTANCE=Element, it is possible to choose between different options for the output magnitudes and units.

CONVERSION FACTOR FROM FILE UNITS TO MeV. When energy points are from a file, this is the conversion factor used to change from user units to xcom units (MeV). This option is useful to create cross section with a grid file from xop/sources saved with the "Write files for xop/optics" option. Use 1e-6 in this case to pass from eV to MeV.

#XOP on-line help file: xyaup.txt

----- file created by xop_makedoc on: Fri Mar 7 13:26:18 2003

----- Documentation for /scisoft/XRayOptics/xop2.1/src_idl/sources/xyaup.pro ---
--

============================ Xyaup ====================================

  Xyaup is a widget based graphical interface to calculate spectra of a
  tapered undulator insertion devices.

  It interfaces the program YAUP 1.3.1 written by B. Boyanov (see Help/Yaup)

 DESCRIPTION OF THE CONTROLS IN THE MAIN WINDOW:

  File:
    XYaup input parameters: This option allows to save the current
                parameters to a file for later loading. It also allows
                to save the current parameters as defaults for being
                used when the application is initialized. In the last
                case, the file is named "application".xop (where
                "application " is the name of the current XOP
                application) and is written in the directory pointed
                by the XOP_DEFAULTS_DIR environment variable (which
                must be set). The parameter file is ASCII and can be
                read and edited with care.
    Yaup file: This option allows to load/write the current parameter
                and result files for further calculations. The used file
                formats are those used by YAUP. Therefore, they
                can be used to run YAUP without the interface or to
                import YAUP files created outside the XYAUP application.
    Write Files for XOP/Optics: Saves the current undulator
                spectrum in the SRCOMPE (flux) and SRCOMPW (Power) files
                to be used for the other XOP application from Optics
                menu.
  Quit and preserve files: Quits without cleaning current directory
                (i.e., preserving the created data files.)
  Quit: to exit from the program

 BField:
                from ASCII file:
                Yaup needs a file with tha magnetic field. This may be
                obtain from a user's file (column-formatted, containing
                three colums: z, B(z), and phi(z), where the z s are
                equidistant with step PERIOD/NPTS.
                See Help/Yaup for definitions of PERIOD and NPTS.
                There should be NPTS*NPER+1 lines in the ASCII file.

                from XBFIELD Preprocessor: calls XBFIELD, an interface for the
                program BFIELD distributed in the YAUP package. This program
                creates the magnetic field starting from the undulator
                oparameters.

                from Linear B field: Creates a magnetic field modulated with a
                straight line with the given B or K extrema.

 Set_Parameters:
  Set Parameters: to define the parameters for the calculation.
                The same result is obtained pressing the "Set Parameters"
                button in the main XYAUP window.
               Please refer to the information under the HELP
                button for a complete description of the parameters. After
                pressing the ACCEPT button, YAUP starts running.
  Set Defaults: Sets the default parameters.

  Show: Display results
                Plot B field: Plots the computed B field.
                Plot Trajectory: Plots the electron trajectory in the

defined magnetic field.
Show Trajectory Numerical Data: display the trajectory output file.
Plot Results: Makes 2-D or 3-D plots of the results, depending on the mode and other defined parameters.
Show Results Numerical Data: display the yaup result file.

Help: Shows the YAUP help and the XYAUP help (this text).

CREDITS:
Published calculations made with XOP should refer:

M. Sanchez del Rio and R. J. Dejus "XOP: Recent Developments" SPIE proceedings vol. 3448, pp.340-345, 1998.

In addition, published calculations using the XYAUP package should also cite:

B. I. Boyanov, G. Bunker, J. M. Lee, and T. I. Morrison "Numerical Modeling of Tapered Undulators" Nucl. Instr. Meth. A339, 596-603, 1994

LAST MODIFICATION: msr/msr/00-07-20

#XOP on-line help file: xyaup_par.txt

Parameters that specify the undulator
=====================================

- PERIOD is the magnet period in centimeters (real)
- NPER is the number of periods (integer, 150 max)
- NPTS is the number of points PER PERIOD at which the trajectory is to be calculated (integer, 10 min, 100 max, 40 sugg.). The magnetic-field modulation and phase-error functions (see eq. 1) must then be given at NPTS points per period (NPTS*NPER-1 points total).

Parameters that define the photon energy range
==

- EMIN is the photon starting energy in eV (real)
- EMAX is the final photon energy in eV (real)
- NE is the number of points in energy at which the spectrum will be calculated (integer, used in spectral calculations, 500 max)

Particle beam parameters
========================

- ENERGY is the electron energy in GeV (real)
- CURRENT is the beam current in Amps (real)
- SIGX is the horizontal beam size in mm (real)
- SIGY is the vertical beam size in mm (real)
- SIGX1 is the horizontal beam divergence in mrad (real)
- SIGY1 is the vertical beam divergence in mrad (real)

Pinhole size and position
=========================

- DISTANCE is the distance to the observation point in meters. If =0 then all pinhole sizes (defined below) are assumed to be in angular units (mrad). Otherwise the pinhole sizes are in millimeters AND ALL BRIGHTNESS/POWER DENSITY DATA IS PER MM^2 RATHER THAN PER MRAD^2, E.G. PH/S/MM^2/0.1%BW.
- XPC is the horizontal position of the pinhole center in mrad or mm (real)
- YPC is the vertical position of the pinhole center in mrad or mm (real)
- XPS is the horizontal pinhole size in mrad or mm (real) - YPS is the vertical pinhole size in mrad or mm (real)
- NXP is the number of pinhole subintervals in the horizontal direction (integer, 100 max)
- NYP is the number of pinhole subintervals in the vertical direction (integer, 100 max)

Control parameters
==================

- MODE=0-7 specifies the calculation mode (integer)
  MODE=0 - trajectory calculation only. The settings of all parameters on lines 2-4 are irrelevant in this case.
  MODE=1 - spectrum of the brightness from EMIN to EMAX at NE points at position XPC,YPC. In this case XPS,YPS, NXP, and NYP are irrelevant (see Section VII).
  MODE=2 - angular distribution of the brightness at EMIN. In this case EMAX and NE are irrelevant.
  MODE=3 - spectral AND angular distribution of the brightness.
  MODE=4 - spectrum of the flux through a pinhole at

NE points in the range [EMIN,EMAX].
MODE=5 − spectral distribution of the radiated power at XPC,YPC. In this mode XPS, YPS, NXP and NYP are irrelevant (see Section VII).
MODE=6 − spectral AND angular distribution of the radiated power.
MODE=7 − angular distribution of the radiated power integrated from EMIN to EMAX. In this case NE determines the number of energy points at which the spectrum will be calculated prior to the integration.

- NSIG is the number of standard deviations of beam divergence to include in the calculation (integer, max=5). NSIG=0 gives the zero−emittance spectrum (in this case SIGX, SIGY, SIGX1, SIGY1 are irrelevant).

- TRAJECTORY is a trajectory−calculation flag
  TRAJECTORY=OLD − read the trajectory from the disk file specified by the keyword TFILE (see below).
  TRAJECTORY=NEW − read the B−field distribution from a file specified by the keyword BFILE and calculate the trajectory without saving it.
  TRAJECTORY=NEW+KEEP − read the B−field distribution from a file specified with the keyword BFILE, calculate the trajectory and store it in a file specified by the keyword TFILE.

- XSYM=YES,NO flags whether horizontal symmetry of the spectrum should be enforced (integer). Vertical symmetry is always enforced. XSYM=NO − do not enforce horizontal symmetry XSYM=YES − enforce horizontal symmetry

- HANNING=0,1,...,NPER/2 is the number of periods at the entrance and exit of the undulator over which a Hanning window will be applied to the solution for the trajectory prior to the FFT. If HANNING=0 no window will be applied (default). USE WITH EXTREME CAUTION.

I/O filename specifications

- BFILE − when TRAJECTORY=NEW or NEW+KEEP this keyword must specify a complete directory specification of the disk file containing the B−field distribution (<80 chars). If TRAJECTORY=OLD the value of BFILE is irrelevant and may be omitted. THE FILE NAME MUST BE ENCLOSED IN DOUBLE QUOTES.

- TFILE − when TRAJECTORY=OLD or NEW+KEEP this keyword must specify a complete directory specification of the disk file containing the trajectory or to which the trajectory will be written. The maximum length of the filenames is 80 characters. THE FILE NAME MUST BE ENCLOSED IN DOUBLE QUOTES. If TRAJECTORY = NEW this keyword may be omitted.

NOTE: unless told otherwise YAUP converts all input to upper case. On case−sensitive systems (e.g. UNIX) this may cause problems with the interpretation of file names. In such cases (or any time you want to keep the file names case−sensitive and/or want to use file names containing blanks) enclose the file names in DOUBLE quotes, e.g. BFILE= "/users/myname/myfile.b"

Miscellaneous keywords

- QUIET=YES,NO − when YAUP encounters a word that it does not recognize it will complain loudly. You may prevent it from doing so by using the QUIET flag. By default QUIET is set to NO. Setting QUIET=YES will cause all unrecognized keywords to be

ignored. It is your responsibility to avoid all typos and accidental occurrences of text containing keywords. It is probably a good idea to set QUIET=NO (default) and comment out all additional text in YAUP.INP

− END − all input following the keyword END is ignored

#XOP on-line help file: yaup.txt

YAUP - Yet Another (Useless) Undulator Program
Version 1.3.1

MODIFICATION RECORD

- 12/92 - Initial version (without FFTs); calculates spectral and angular distributions of the brightness and flux through pinholes.
- 01/92 - FFT version.
- 04/92 - Bugs in module EXTRCT and trajectory calculation fixed. Added degree-of-linear-polarization calculations.
- 06/92 - Add Hanning windows to reduce spectral leakage; expert-user options; power-load calculations.
- 10/92 - New input-file format. Life is easy now.(v1.0)
- 04/93 - Include particle beam sizes. (v1.1)
- 09/93 - Fix a bug in the flux calculations with finite observation distance Some changes in the input file format. (v1.1b)
- 11/93 - Switch back to double precision variables for temp storage. Increases RAM requirements but improves "inter platform" reproducibility of the results. (v1.2) Check (but do not enforce) L/R symmetry criterion. (v1.2b) More flexible scratch file names. (v1.2c)
- 12/93 - User-definable scratch file names. Bug in spline interpolations fixed (INTGRD). Add GNUPLOT and BASENAME. (v1.2d)
- 04/94 - Fix imsc bug. Rewrite parser routines. Now compiles and runs on an IBM RISC/6000 cluster. (v1.3)
- 04/94 - Fix minor output bugs in mode 7. Fix integration bug in mode 7 (v1.3.1)
- 07/94 - Some adjustments to the user interface (v 1.3.2)

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REFERENCE

B. I. Boyanov, G. Bunker, J. M. Lee, and T. I. Morrison
"Numerical Modeling of Tapered Undulators"
Nucl. Instr. Meth. A339, 596-603, 1994

DISCLAIMER

Now that this junk is out of the way let’s get on with the fun stuff.

TABLE OF CONTENTS

I. INTRODUCTION

> 1 yawp or yaup \’yoÇp\ vi
> [ME yolpen]
> (14c)
> 1: to make a raucous noise: SQUAWK
> 2: CLAMOR, COMPLAIN
> Ð yawp–er n
>
> 2 yawp also yaup n
> (1824)
> 1: a raucous noise: SQUAWK
> 2: something suggestive of a raucous noise; specif:
> rough vigorous language
>
> yawp (or yaup) vb
> 1 syn SQUALL 1, caw, ||quawk, squak, squawk
> 2 syn GRIPE, ||beef, ||bellyache||||bitch, bleat,
> ||blow off, crab, fuss, squawk, yammer
>
> Webster’s Ninth New Collegiate Dictionary
> Webster’s Collegiate Thesaurus
> First Digital Edition
> Copyright (c) 1988, 1990
> NeXT Computer, Inc.,
> and Merriam–Webster Inc.

YAUP (Yet Another (Useless) Undulator Program) is a program that calculates radiation patterns (spectral and angular distributions of the brightness, the flux through a pinhole, spectral and angular power distributions) and polarization properties of tapered and untapered undulator radiation. The program has the following capabilities and restrictions:

– the magnetic field B within the undulator is assumed to be a vertically–polarized amplitude and/or frequency–modulated sinusoid. The B–field distribution is read in from an external file. Random and or systematic errors in the magnitude and phase of the field may be included.

– e–beam size and divergence may be included in a first–order approximation as a convolution of the zero–emittance spectrum with the e–beam distribution.

– up–down (vertical) symmetry of the angular distribution of the brightness is always assumed but left–right (horizontal) symmetry of the spectrum may or may not be enforced (see the description of input parameter XSYM in sections IV and VII).

- besides tapered undulators the program may be used to calculate distributions from untapered undulators. These calculations, however, are inefficient and programs designed specifically for untapered undulators, e.g. URGENT and USER_UNDULATOR, are usually much faster. We recommend that the program be used for untapered undulators at energies not higher than the fifth harmonic only when field errors have to be accounted for (see section VII).

- The use of FFTs greatly enhances the performance of the program (in terms of time needed to complete the calculation), especially in the case of calculations in a broad spectral range.

II. COMPILATION INSTRUCTIONS

YAUP is written in FORTRAN and uses several non-standard but widely available extensions - mainly DO ... END DO and DO WHILE ... END DO constructions, COMPLEX*16 data types and its associated intrinsic functions, and INCLUDE statements. It calls no external library routines so it should be fairly easily transportable. With the exception of (a large number of) insignificant warnings it passes all FTNCHEK tests with flying colors.

As of this writing YAUP has been tested on the following machines:

* NeXTStation (black), Absoft 3.1 compiler (BSD UNIX 4.3)
* VAX 3100-3600, DEC FORTRAN compiler (VMS 5.1 or later)
* Macintosh Quadra 610, Language Systems 3.0 compiler (System 7.1)
* IBM RISC System/6000 cluster, IBM AIX XL Compiler/6000 (IBM AIX 3.2)

The program is distributed as a single module named YAUP.F. The file YAUP.INC is an include file that contains definitions of essential parameters and common blocks and should be placed in the same directory as YAUP.F at the time of compilation.

THE PROGRAM SHOULD BE COMPILED WITH THE STATIC MEMORY OPTION TURNED ON. IF YOUR COMPILER IS CASE SENSITIVE IT IS SAFER TO FOLD ALL VARIABLE NAMES TO LOWER (OR UPPER) CASE. BEWARE OF OPTIMIZING COMPILERS - THE "OPTIMIZATIONS" MAY LEAD TO IMPROPER EXECUTION AND SHOULD BE AVOIDED UNLESS YOU ABSOLUTELY TRUST YOUR COMPILER'S OPTIMIZER. THE FIRST THING YOU SHOULD DO IF YAUP DOES NOT EXECUTE PROPERLY IS TURN OFF ALL OPTIMIZATIONS.

A VERY important parameter in YAUP.INC that may need customizing to your compiler is LWORD. YAUP uses unformatted direct-access files to store intermediate results and the various FORTRAN compilers handle these files in different ways. Generally the value of LWORD should be set equal to the number of bytes in the direct-access storage unit, which for most compilers is 1. The VAX FORTRAN compilers, however, use 4-byte portions (words). SET LWORD TO 4 PRIOR TO COMPILATION IF YOU USE VAX FORTRAN OR SOME OTHER COMPILER WITH FUNNY IDEAS ON HOW THE RECL LENGTHS SHOULD BE SPECIFIED. The program is distributed with LWORD set to 1. It should run on any system with this setting but the amount of free disk space needed for successful execution may be unnecessarily large.

Some compilers (such as the older versions of MacFortran) do not allow direct-access records longer than 1024 bytes. YAUP may not run on such systems.

Another possible customization concerns the way your compiler handles output string editing. YAUP prints information on the progress of the calculations to the screen and in doing so it uses '+' (overprint) character editing. If your compiler interprets the first character of the output string as a control character you need not do anything (VAX and MPW (LangSys) FORTRAN, for example). If this is not so, special

action may be required (this is the case with many, if not most, Unix compilers). Absoft FORTRAN for NeXTStep, for example, requires the statement

```
OPEN(UNIT=6,ACTION='PRINT')
```

added to the very beginning of YAUP.F to ensure that the screen-directed output is handled properly. Check your compiler manula and inser the appropriate code if necessary.

YAUP needs somewhat large amounts of RAM and free disk space to compile and run properly. At least 8 Mb RAM are needed for compilation on most machines, 5-6 Mb of free RAM should be available at runtime, and UP TO 260 Mb of free disk space (for temporary data storage) may be needed IF THE PROGRAM IS PUSHED TO EXTREMES. The amount of disk space needed depends on the input parameters, but approximately 2*8*NXP*NYP*NE bytes of disk space will be needed for temporary data storage (for a description of NXP, NYP and NE see section IV). If anything, this is a very rough underestimate.

For FORTRAN gurus only: The FORTRAN compiler on AIX machines handles IOSTAT in a very weird fashion. When an I/O error is encountered, e.g. attempt to read a characted where a number is expected, IOSTAT is not set to a non-zero value, as is the case with most other compilers I have had to deal with. Instead, an error message is printed to the terminal and the error is ignored. This interferes with YAUP's internal error-checking routines. If someone knows of a fix, e.g. a compiler switch, I'd like to hear about it. Send email to boyan@tmnxt1.iit.edu.

III. NEW FEATURES

This section describes the new features in YAUP relative to version 1.2. Skip this section if this is the first time you are using YAUP.

- The L/R symmetry criterion (see B. I. Boyanov et al., NIM A, Feb 1, 1994) is checked, but not enforced. That means that the program will warn you when you are using XSYM=YES at dangerously high energies, but will not force you to switch to XSYM=NO.

- New keywords: BASENAME, GNUPLOT. See section IX.

- A serious bug in the spline interpolation procedures has been fixed. The bug caused problems in calculations with large values of NXP and/or NYP only.

- A bug in the I/O routines has been fixed. (imsc -> imisc conflict)

- The parser routines have been rewritten and are hopefully more robust. There are no changes in the input file format and the user interface.

- The behavior of the program in MODE 7 has been fixed up.

- NXP and NYP are no longer under user control in MODE 1 and may be set automatically in other modes.

- The default value of UPDATE is 1 (i.e. UPDATE=0 defaults to UPDATE=1). Use UPDATE=-1 to turn off updating.

IV. INPUT FILE FORMAT

In the rest of this document keywords and file names are shown capitalized. This is done for clarity and is not required. If you are using YAUP on a system with case-sensitive file names (e.g. UNIX) use LOWER CASE for the file names. The case of the keywords is irrelevant as the program capitalizes all input internally.

Input is read from the file YAUP.INP which is expected to be in the current directory. The input consists of tab, space or comma−delimited keywords followed by values. On any given line in the input file all text that appears after any of the characters %,!,#, or ; is treated as a comment (ignored).

The values are separated from the keywords by one or more spaces, tabs equal signs. A list of valid keywords follows :

```
PERIOD, NPER, NPTS
EMIN, EMAX, NE
ENERGY, CURRENT, SIGX, SIGY, SIGX1, SIGY1
DISTANCE, XPC, YPC, XPS, YPS, NXP, NYP
MODE, NSIG, TRAJECTORY, XSYM, HANNING
BFILE, TFILE
QUIET,END
```

The order in which the keywords appear in YAUP.INP is not important (as long as ALL keywords are defined) but for the sake of clarity they may be grouped in the following categories :

LINE 1 : specifies the undulator

- PERIOD is the magnet period in centimeters (real)
- NPER is the number of periods (integer, 150 max)
- NPTS is the number of points PER PERIOD at which the trajectory is to be calculated (integer, 10 min, 100 max, 40 sugg.). The magnetic−field modulation and phase−error functions (see eq. 1) must then be given at NPTS points per period (NPTS*NPER−1 points total).

LINE 2 : defines the photon energy range

- EMIN is the photon starting energy in eV (real)
- EMAX is the final photon energy in eV (real)
- NE is the number of points in energy at which the spectrum will be calculated (integer, used in spectral calculations, 500 max)

LINE 3 : particle beam parameters

- ENERGY is the electron energy in GeV (real)
- CURRENT is the beam current in Amps (real)
- SIGX is the horizontal beam size in mm (real)
- SIGY is the vertical beam size in mm (real)
- SIGX1 is the horizontal beam divergence in mrad (real)
- SIGY1 is the vertical beam divergence in mrad (real)

LINE 4 : pinhole size and position

- DISTANCE is the distance to the observation point in meters. If =0 then all pinhole sizes (defined below) are assumed to be in angular units (mrad). Otherwise the pinhole sizes are in millimeters AND ALL BRIGHTNESS/POWER DENSITY DATA IS PER MM^2 RATHER THAN PER MRAD^2, E.G. PH/S/MM^2/0.1%BW.
- XPC is the horizontal position of the pinhole center in mrad or mm (real)
- YPC is the vertical position of the pinhole center in mrad or mm (real)
- XPS is the horizontal pinhole size in mrad or mm (real) − YPS is the vertical pinhole size in mrad or mm (real)
- NXP is the number of pinhole subintervals in the horizontal direction (integer, 100 max)
- NYP is the number of pinhole subintervals in the vertical direction (integer, 100 max)

LINE 5 : control parameters

- MODE=0−7 specifies the calculation mode (integer)
  MODE=0 − trajectory calculation only. The settings of all parameters on lines 2−4 are irrelevant in this case.
  MODE=1 − spectrum of the brightness from EMIN to EMAX at NE points at position XPC,YPC. In this case XPS,YPS, NXP, and NYP are irrelevant (see Section VII).
  MODE=2 − angular distribution of the brightness at EMIN. In this case EMAX and NE are irrelevant.
  MODE=3 − spectral AND angular distribution of the brightness.
  MODE=4 − spectrum of the flux through a pinhole at NE points in the range [EMIN,EMAX].
  MODE=5 − spectral distribution of the radiated power at XPC,YPC. In this mode XPS, YPS, NXP and NYP are irrelevant (see Section VII).
  MODE=6 − spectral AND angular distribution of the radiated power.
  MODE=7 − angular distribution of the radiated power integrated from EMIN to EMAX. In this case NE determines the number of energy points at which the spectrum will be calculated prior to the integration.

- NSIG is the number of standard deviations of beam divergence to include in the calculation (integer, max=5). NSIG=0 gives the zero−emittance spectrum (in this case SIGX, SIGY, SIGX1, SIGY1 are irrelevant).

- TRAJECTORY is a trajectory−calculation flag
  TRAJECTORY=OLD − read the trajectory from the disk file specified by the keyword TFILE (see below).
  TRAJECTORY=NEW − read the B−field distribution from a file specified by the keyword BFILE and calculate the trajectory without saving it.
  TRAJECTORY=NEW+KEEP − read the B−field distribution from a file specified with the keyword BFILE, calculate the trajectory and store it in a file specified by the keyword TFILE.

- XSYM=YES,NO flags whether horizontal symmetry of the spectrum should be enforced (integer). Vertical symmetry is always enforced. XSYM=NO − do not enforce horizontal symmetry XSYM=YES − enforce horizontal symmetry

- HANNING=0,1,...,NPER/2 is the number of periods at the entrance and exit of the undulator over which a Hanning window will be applied to the solution for the trajectory prior to the FFT. If HANNING=0 no window will be applied (default). USE WITH EXTREME CAUTION.

LINE 6 : I/O filename specifications

- BFILE − when TRAJECTORY=NEW or NEW+KEEP this keyword must specify a complete directory specification of the disk file containing the B−field distribution (<80 chars). If TRAJECTORY=OLD the value of BFILE is irrelevant and may be omitted. THE FILE NAME MUST BE ENCLOSED IN DOUBLE QUOTES.

- TFILE − when TRAJECTORY=OLD or NEW+KEEP this keyword must specify a complete directory specification of the disk file containing the trajectory or to which the trajectory will be written. The maximum length of the filenames is 80 characters. THE FILE NAME MUST BE ENCLOSED IN DOUBLE QUOTES. If TRAJECTORY = NEW this keyword may be omitted.

NOTE: unless told otherwise YAUP converts all input to upper case. On

case-sensitive systems (e.g. UNIX) this may cause problems with the interpretation of file names. In such cases (or any time you want to keep the file names case-sensitive and/or want to use file names containing blanks) enclose the file names in DOUBLE quotes, e.g. BFILE= "/users/myname/myfile.b"

LINE 7: Miscellaneous keywords

- QUIET=YES,NO - when YAUP encounters a word that it does not recognize it will complain loudly. You may prevent it from doing so by using the QUIET flag. By default QUIET is set to NO. Setting QUIET=YES will cause all unrecognized keywords to be ignored. It is your responsibility to avoid all typos and accidental occurrences of text containing keywords. It is probably a good idea to set QUIET=NO (default) and comment out all additional text in YAUP.INP

- END - all input following the keyword END is ignored

EXAMPLE 1. Here is a sample input file

```
----------------------YAUP.INP begins here-------------------
;Magnet parameters
period=3.3      NPER = 75       npts=20

#Photon energy
Emin=4000.  eMax = 6000.        nE=300  ;you may mix cases as you wish

%Storage ring
ENERGY=7.0              CURRENT=0.1
SIGX=0.308              SIGY=0.085
SIGX1=0.024             SIGY1=0.009

!Pinhole (mm or mrad)
DisTaNcE = 50. ; all pinhole sizes are in mm now,
               ; case of keyword does not matter
XPC=0.000       XPS=2.000       NXP=50    ; this text is ignored
YPC=0.000       YPS=2.000       NYP=50

%Calculation parameters
MODE=4          NSIG=2  TRAJECTORY=NEW
XSYM=yes        HANNING=0

;Filenames
BFILE = "test.b"
;TFILE = "test.trj"

END

Note that four types of comment characters are allowed, even in the
middle of a line.  You may put anything your heart desires after an
END statement without using any comment characters, just like this
text.
----------------------YAUP.INP ends here-------------------
```

In this case TRAJECTORY=NEW (calculate without saving), so there is no need to specify TFILE. Note that comments may appear anywhere in the input file and that empty lines are ignored. Care must be taken to avoid comments which are identical to keywords when QUIET=YES.

EXAMPLE 2. Another input file

```
----------------------YAUP.INP begins here-------------------

;Magnet parameters
PERIOD=3.3      NPER = 75       NPTS=20
```

```
;Photon energy
EMIN=4000.  EMAX = 6000.        NE=300

;Storage ring
ENERGY=7.0              CURRENT=0.1
SIGX=0.308              SIGY=0.085
SIGX1=0.024             SIGY1=0.009

;Pinhole (mm or mrad)
DISTANCE = 0.  ; all pinhole sizes are now in mrad
XPC=0.000       XPS=0.000       NXP=0
YPC=0.000       YPS=0.100       NYP=50

;Calculation parameters
MODE=2          NSIG=2  trajectory=NEW+KEEP
XSYM=yes        HANNING=0

;Filenames
BFILE = "test.b"
TFILE = "test.trj"

--------------------YAUP.INP ends here-------------------
```

Here TRAJECTORY=NEW+KEEP (calculate and save) so both input (for the B−field) and output (for the trajectory) filenames must be specified. The same is true if MODE=0 regardless of the setting of TRAJECTORY Note that you may omit the END keyword when you don’t need it.

EXAMPLE 3. Yet another sample input file.

```
-------------------YAUP.INP begins here-------------------

;Magnet parameters
PERIOD=3.3      NPER = 75       NPTS=20

;Photon energy
EMIN=4000.  EMAX = 6000.        NE=300

;Storage ring
ENERGY=7.0              CURRENT=0.1
SIGX=0.308              SIGY=0.085
SIGX1=0.024             SIGY1=0.009

;Pinhole (mm or mrad)
DISTANCE = 50.
XPC=0.000       XPS=0.100       NXP=50
YPC=0.000       YPS=0.100       NYP=50

;Calculation parameters
MODE=4          NSIG=2  TRAJECTORY=old
XSYM=yes        HANNING=0

;Filenames
BFILE = "testbri"
TFILE = "test.trj"

--------------------YAUP.INP ends here-------------------
```

EXAMPLE 4. A bad example

```
-------------------YAUP.INP begins here-------------------
QUIET=yes

Magnet parameters − this will not cause an error
PERIOD=3.3      NPER = 75       NPTS=20

;Photon energy
EMIN=4000.  EMAX = 6000.        NE=300
```

```
QUIET=no
Storage ring − this text will make YAUP complain
ENERGY=7.0              CURRENT=0.1
SIGX=0.308              SIGY=0.085
SIGX1=0.024             SIGY1=0.009

;Pinhole (mm)
DISTANCE = 50.
XPC=0.000       XPS=0.000       NXP=0
YPC=0.000       YPS=0.100       NYP=0

;Calculation parameters
MODE=1          NSIG=2  TRAJECTORY=old
XSYM=yes        HANNING=0

; MODE=1 so YPS does not matter

;Filenames
BFILE = "test.b"
TFILE = "test.trj"

−−−−−−−−−−−−−−−−−−−YAUP.INP ends here−−−−−−−−−−−−−−−−−−
```

In this example QUIET is initially set to YES so the line "Magnet parameters..." will be ignored. Later in the file, however, QUIET is set back to NO and the line "Storage..." will cause the program to complain.

Extensive error checking of the input stream is performed but it is mostly for syntax errors and missing keywords. Obvious errors like negative ENERGY or variables out of bounds will be reported but no other attempt is made to see if the input data makes any sense.

V. OUTPUT FILE FORMAT

All results are written to a file called YAUP−N.OUT where N is an integer from 0 to 9. Initially the program tries to open a file called YAUP−0.OUT. If the file already exists in the current directory the program attempts to open the file YAUP−1.OUT and so on, until a unique file name YAUP−N.OUT if found. If the files YAUP−0.OUT through YAUP−9.OUT already exist the program terminates with the error message

```
*************
opnout:: cannot open an output file
please delete all yaup−*.* files
*************
```

You will have to manually delete at least one of the YAUP−*.OUT files before attempting to restart the program. This inconvenience is intended to protect the results of lengthy calculations from accidental deletion (you can tell that I did that many times, can't you :−)).

The output file is straight ASCII and may be plotted with the program of your choice.

VI. PROGRAM DESCRIPTION

The program assumes that the tapered undulator is a periodic array of magnets with alternating poles and a magnet gap that varies along the undulator axis z in a user−specified fashion. Thus the magnet field within the undulator is some amplitude−modulated sinusoid :

$$B_{tot}(z)=B(z)*\sin(2*\pi/L*z+\phi(z)). \qquad (1)$$

Here Btot is the total field, z is the longitudinal coordinate (along the undulator axis), L is the undulator period and phi(z) accounts for any phase errors that may be present in the field (amplitude errors should be included in B(z)).

The user specifies the function B(z) (in tesla) and phi(z) (in radians). The equations of motion are solved numerically subject to the boundary condition that the transverse displacement at z=0 and z=N*L is zero (no beam steering). Zero beam divergence is assumed in these calculations.

Once the trajectory is available it is used to calculate the energy radiated by a single electron traversing that trajectory in a user−specified angular and energy range. In order to minimize the computation time the program tries to use certain symmetries of the spectrum to reduce the angular range to the possible minimum. It is therefore very likely that the angular range of the actual calculations (printed on the screen) will differ significantly from the angular range requested by the user, but as long as the FINAL results are in the requested range this should be no cause for alarm.

As mentioned earlier beam emittance may be accounted for in a first order approximation by convoluting the zero emittance spectrum with the e−beam velocity distribution. Up to five standard deviations of beam divergence may be included in the calculations at this time which should be more than enough for all practical purposes.

VII. HINTS AND SUGGESTIONS (PLEASE, PLEASE READ)

If a pinhole covers both positive and negative angles the program may not calculate the brightness over the requested angular range but will rather use the allowed reflection symmetries of the spectrum to minimize the angular range of the calculations. In such case there will be APPROXIMATELY (see below) NXP/2 and NYP/2 points in the minimal angular range. Any adjustments to the input parameters are written to the output file so that the values saved there reflect the ACTUAL parameters used in the calculations.

The parameter XSYM flags whether to assume reflection symmetry of the spectrum with respect to the vertical (yz) plane. This is a valid symmetry for untapered undulators (if no field errors are present). In every other case the presence or absence of this symmetry should be verified (calculate an angular distribution of the brightness at several energies with XSYM=NO for an on−axis pinhole and compare the results for positive and negative x−angles) and XSYM=YES should be used whenever possible. For an approximate analytical criterion see the reference cited at the beginning of this document. This criterion is checked internally and whenever it is not satisfied and XSYM is set to YES the program will issue a warning message:

```
**********************************************
*EMAX may be too high.  Consider using XSYM=NO.*
**********************************************
```

In order to calculate the convolutions with the beam divergence efficiently (NSIG>0, all modes), the step sizes for the brightness calculations and the sampling of the e−beam distribution have to be identical and fixed. Since the number of sampling points for the particle beam distribution is limited to 78 in each direction, some minor adjustment of the step and pinhole sizes may be needed. The program performs all necessary adjustments to NXP, NYP, XPS and YPS automatically and saves them in the output file. The values written to the output file are the ones used in the calculation.

Since the user−requested pinhole must be covered in an integer number of steps minor adjustments to the pinhole sizes may also be necessary. This is done automatically and all changes are recorded in

the output file.

To account properly for beam emittance (NSIG>0) the program needs a "sufficiently dense" angular/spatial mesh of points. This is especially true for calculations involving untapered undulators and tapered undulators with a small amount of taper, where the zero−emittance spectrum is a rapidly oscillating function of the angle between the observation direction and the undulator axis. An angular/spatial mesh may be considered "sufficiently dense" if doubling the number of points in angle in the X and/or Y directions (i.e. NXP and NYP) leaves spectrum reasonably unchanged. Insufficiently dense angular/spatial mesh will result in spurious oscillations in the calculated spectra.

Usually NSIG=2 will do a decent job and NPTS=40 is more than enough. Unnecessarily large values for these parameters will slow down the execution of the program considerably and may lead to insufficient averaging (and smoothing) of the zero− emittance spectrum.

If NXP and/or NYP=0,1 and XPS and/or YPS>0, the stepsize for the angular−distribution calculations is chosen internally. It is highly recommended that you set NXP and NYP to zero when MODE=2,3,4,6. Note that when MODE=1,5 XPS and YPS are forced to zero and the angular stepsize is ALWAYS controlled internally (if NSIG>0).

It is a good idea to leave a blank line at the end of the input file. If this is not done the program may respond with an error message on some systems.

Only minor error checking of the input stream is performed. If inconsistent input parameters are given the results produced by the program (if any) most likely will make no sense. It is the user’s responsibility to ensure that the input is "reasonable" and the output behaves "as expected" to certain changes of the input parameters. THIS IS NOT A COMMERCIAL PRODUCT AND IS NOT DESIGNED TO BE "FOOL−PROOF".

As mentioned in the introduction, it is not recommended to use this program for calculations of untapered undulators. URGENT will handle such devices much more efficiently. Programs such as URGENT, however, cannot account for field errors or fringe fields of any kind. If this is what you want, YAUP may be used to do the calculations but it must be kept in mind that the zero−emittance spectrum of untapered undulators is a wildly oscillating function of the angles (both horizontal and vertical) and in some cases the convolution with the beam emittance may not provide sufficient "statistics" to wash out these oscillations unless the stepsize is sufficiently small (this is especially true for large values of NSIG and/or XPS/YPS when MODE=2,3,4,6). In such cases it is HIGHLY desirable that you set NXP=NYP=0 and NSIG=2 whenever possible. If you insist on using your own NXP/NYP, please run YAUP once with NXP=NYP=0 and note the step sizes (in both the X and Y directions) that the program chooses. We recommend that the step sizes for all subsequent calculations with this configuration (i.e. number of poles, magnet period, beam energy, AND photon energy range) does not exceed these values more than two times whenever possible.

Use HANNING *very* cautiously. When in doubt use HANNING=0. Whenever HANNING>0 *always* inspect the trajectory visually.

When interrupted the program leaves the internal files YAUP.CFG, YAUP.S0, and YAUP.S1 on the disk. These files must be removed manually before restarting the program. For more info see section IX.

In some cases the program will terminate with an error message suggesting that you use certain values of NCRIT and/or MFFT. (see section IX). Under normal operation (i.e. when you are not abusing the program) they will not be encountered. If you use the suggested values the program will probably produce results but you should be ** VERY VERY ** SUSPICIOUS of them.

VIII. DATA FILE FORMATS

The B-field file should be written in double precision to an unformatted FORTRAN file as follows :

```
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        .
        .
        .
        NPTST=NPER*NPTS+1
        DZ=PERIOD/NPTS
        BMIN=1.D30
        DO I=1,NPTST
           Z=(I-1)*DZ
           < calculate B(z) and phi(z) >
           IF (B(I).LT.BMIN) BMIN=B(I)
        END DO
        OPEN(1, FILE=filename, STATUS='UNKNOWN',FORM='UNFORMATTED')
        WRITE (1) PERIOD, NPER, NPTS,BMIN
        WRITE(1) ( B(I), PHI(I), I=1,NPTST )
        CLOSE(1)
        .
        .
        .
```

In the above code NPTST is the total number of points at which the trajectory will be calculated, PERIOD is the undulator period (in cm)), and B (in tesla) and PHI are the values of the modulating function and the phase errors (as defined by eq.(1)) at points Z=(I-1)*DZ, I=1,NPTST, DZ=PERIOD/NPTS. BMIN is the minimum value of B(I), I=1,...,NPTST. The values of PERIOD, NPER and NPTS in the B-field file and YAUP.INP must be the same or the program will terminate with an error message.

A program called BFIELD.F is distributed with YAUP.F. BFIELD.F is a standalone module that generates a B-field file for an undulator with a linearly tapered gap in a format acceptable to YAUP. The user must specify the gap GZMIN at Z=Zmin=0 and the amount of gap taper DG=(GZMAX-GZMIN)/GZMIN (either positive or negative). The program interpolates the gap linearly between GZMIN and GZMAX. The field strength dependence is specific to the proposed APS undulators but the user may modify this section of the program according to his/her specific needs. Zero phase errors are assumed. See the file BFIELD.F for more details.

The format of the trajectory file is similar to that of the B-field file. YAUP uses the following code to save the trajectory (when ITRAJ=SAVE or MODE=0) :

```
        IMPLICIT DOUBLE PRECISION (A-H,O-Z)
        .
        .
        .
        KMIN=0.934*PERIOD*BMIN
        EFUND=949.*ENERGY**2/(PERIOD*(1.D0+KMIN**2/2.D0))
        OPEN(1, FILE=filename,STATUS='UNKNOWN',FORM='UNFORMATTED')
        WRITE(1) PERIOD,NPER,NPTS,ENERGY,EFUND
        WRITE(1) ( CT(I),X(I),BETAX(I),BETAZ(I), I=1,NPTST )
        CLOSE(1)
        .
        .
        .
```

where PERIOD,NPER,NPTS,and NPTS are as before, ENERGY is the electron energy in GeV, EFUND is the on-axis fundamental energy (in eV) of a untapered undulator with K=KMIN=0.934*PERIOD*BMIN, and CT (in centimeters), X (in cm), BETAX, and BETAZ are the usual quantities as a function of the longitudinal coordinate Z=(I-1)*DZ, I=1,NPTST.

Contact the authors at the addresses given at the end of this document if you need a program that converts the trajectory and B-field files back to ASCII format and vice-versa.

IX. "EXPERT" options.

This section deals with somewhat technical questions that concern primarily the fine-tuning of the program execution. It is intended for "expert" users. The use of the capabilities described here is strictly optional. If you intend to use the program as a black box you probably do not need to read what follows.

The execution of YAUP is controlled by a number of parameters: STATUS, UPDATE, RESOLUTION, NCRIT, MFFT, BW, and GNUPLOT. The most time-consuming portion of the program is the calculation of the zero-emittance Stoke's coefficients S0 and S1. The values of these coefficients as a function of energy and angle are written to two files named YAUP.S0 and YAUP.S1 (defaults). The status of the current job is saved in the "status file" YAUP.CFG. If the program is interrupted at any time, these three files (and the ORIGINAL YAUP.INP) may be used to continue the calculations from the point of interruption instead of starting from scratch. The default location of these files is the current directory. If you would prefer to have them in a scratch directory (e.g. /tmp on UNIX systems) or rename them altogether, you may do so through the use of the BASENAME keyword (see below). On some systems you can avoid counting these files against your disk quota by doing this.

- BASENAME="filespec", if present, determines the basename of all output files produced by YAUP. Here "filespec" is a file specification (enclosed in double quotes as usual) such that "filespec.txt" is a valid file name. Examples of valid filespec's are "/tmp/yaup" (UNIX), "c:\tmp\yaup1" (DOS), "[.junk]yaup2" (VMS), "HD20:junk:yaup3" (Mac). If a basename is given program output will be directed to the file "filespec-n.out" (instead of YAUP-n.OUT), the Stokes' coefficients will be written to "filespec.s0" and "filespec.s1" (instead of YAUP.S0 and YAUP.S1), and the configuration file name will be "filespec.cfg" (instead of YAUP.CFG). This is particularly useful if you want to run several YAUP (batch) jobs in the same directory. Note, however, that input is ALWAYS read from YAUP.INP.

- The handling of YAUP.S0, YAUP.S1 and YAUP.CFG (which will be jointly referred to as "temporary files") is controlled by the STATUS keyword:

  STATUS=NEW - start a new job. Delete all temporary files when done.
  STATUS=NEW+KEEP - start a new job. Keep all temporary files when done.
  STATUS=OLD - continue an interrupted job from the point of interruption. All temporary files must already exist on disk and are deleted at the end of the job.
  STATUS=OLD+KEEP - continue an interrupted job from the point of interruption. All temporary files must already exist on disk and are saved at the end of the job.

If the files were intentionally saved (with STATUS=%%%+KEEP), program execution will resume with the 2D convolution with the beam emittance. You may use this option to calculate the flux through a pinhole once you have calculated the spectral and angular distributions of the brightness in the pinhole (and vice versa). If the file YAUP.INP differs in any way (besides the values of MODE, TRAJECTORY, STATUS, and UPDATE) from the original, the program will terminate with the message

```
*************
status:: invalid checksum found in "yaup.cfg"
```

cannot continue
****

If STATUS=NEW or NEW+KEEP and any of the files YAUP.S0, YAUP.S1, and YAUP.CFG already exist in the current directory the program will terminate with an error message. You will be expected to delete these files manually.

- UPDATE controls the frequency with which the temporary files are updated (i.e. closed and then reopened). If UPDATE>=0 the actual frequency of the updates will depend on the input parameters but approximately every UPDATE*NYP points the files will be closed and then reopened. In the special case NXP/NYP=0 (see section VII) the program will calculate the values of NXP/NYP internally and will update the temporary files every UPDATE*NYP points. When UPDATE<0 an update is forced only once − when the zero−emittance calculations are completed (there may be other unforced updates but that depends on the amount of temporary data and the size of the file buffers on your system). A small (positive) value of UPDATE will force frequent updates and will minimize the data loss in case of a power failure or unintended interruption but will slow down program execution somewhat. Obviously the highest update frequency corresponds to UPDATE=1. UPDATE=0 defaults to UPDATE=1.

- RESOLUTION controls the internal scaling of the angular/spatial stepsize when NXP/NYP=0 (see section VII). The program calculates the angular width ANGW of the zero−emittance first−harmonic lobe of an untapered undulator with the same hardware parameters tuned to EMAX and sets the angular stepsize to ANGW/RESOLUTION. The default is RESOLUTION=6.

- In order to avoid power−aliasing problems YAUP will try to increase the sampling rate of the function that is FFTd until the Nyquist energy is at least ECRIT=NCRIT/2*EFUND+EMAX eV, where NCRIT is a parameter currently set to 20 and EFUND is defined in section VIII. The spurious contributions to the spectrum at any energy E the will then come from energies not lower than E+NCRIT*EFUND. By default NCRIT=20. This means that for untapered undulator calculations the power aliasing contributions will come from harmonics at least 20 orders higher than the highest harmonic in the energy range of interest. In plain English, if you are calculating the undulator spectrum in an energy range containing the fifth, sixth, and seventh harmonic, the power aliasing contributions will come at most from the 27th harmonic.

- To account for the beam emittance the program convolutes the angular distribution of the brightness at each energy with the electron divergence/spatial distribution. Since the energy stepsize in energy of the FFTd spectrum varies with the observation direction the spectrum must be interpolated so as to find the values of the zero− emittance brightness at the user−requested energies. Typically the zero−emittance spectrum of the brightness is a sinc−like oscillating function of energy and a good interpolation will be possible only if the energy mesh is "sufficiently dense". The program controls the energy stepsize of the FFT internally (it has nothing to do with the user−specified energy stepsize as determined from EMIN, EMAX, and NE). The choice for an energy stepsize is based on the values the parameters MFFT and NCRIT and is adjusted so that there will be approximately MFFT points per oscillation in the spectrum. MFFT must be chosen so that a sufficient number of points is available to perform the interpolation described above. The default value is 8. Anything less than 4 seems unacceptable (to me). MFFT MUST BE A POWER OF 2. THE PROGRAM DOES NOT CHECK THAT.

- BW is the bandwidth of the results. The defaults is BW=0.001

(e.g. ph/s/0.1% BW(/mrad^2 or /mm^2))

- GNUPLOT=XLINES,YLINES,NONE allows formatting of the output file for GNUPLOT compatibility. When plotting Z=F(X,Y) 3D data GNUPLOT requires that each set of lines in the input file that defines a contour in the XY plane be separated from the preceding and following sets by a blank line. Obviously this option is useful only when calculating 2D distributions.

  XLINES − a blank line will be left after every NXP*NYP lines.
  YLINES − a blank line will be left after every NYP lines
  NONE − no additional formatting is performed. This is equivalent to omitting the GNUPLOT keyword.

In some cases the program will terminate with an error messages suggesting that you use certain values of NCRIT and/or MFFT. Under normal operation (i.e. when you are not abusing the program) they will not be encountered. If you use the suggested values the program will probably produce results but you should be ** VERY VERY ** SUSPICIOUS of them.

EXAMPLE 5. A demo YAUP.INP that uses the expert options.

```
----------------------YAUP.INP begins here-------------------

;Magnet parameters
PERIOD=3.3      NPER = 75       NPTS=20

;Photon energy
EMIN=3000.  EMAX = 600000.        NE=300

;Storage ring
ENERGY=7.0              CURRENT=0.1
SIGX=0.308              SIGY=0.085
SIGX1=0.024             SIGY1=0.009

;Pinhole (mm or mrad)
DISTANCE = 0.
XPC=0.050       XPS=.100       NXP=50
YPC=0.030       YPS=.100       NYP=50

;Calculation parameters
MODE=4          NSIG=2  TRAJECTORY=old
XSYM=yes                HANNING=0

;Filenames
BFILE = "planar-1.76-bf"
TFILE = "planar-1.76-trj"
BASENAME = "/tmp/hello"

;END

;Advanced keywords
STATUS=old+keep         UPDATE=2          RESOLUTION=12
NCRIT=25                MFFT=0            BW=0.01
----------------------YAUP.INP ends here-------------------
```

In this hypothetical input file STATUS=old+save, UPDATE=2, RESOLUTION=12, NCRIT=25, MFFT1=8 (default), and BW=0.01 (1%BW). Setting any parameter equal to zero signals the program to use the defaults (as defined in the parameter descriptions above). Here BASENAME="/tmp/hello" so output will be written to /tmp/hello-0.out and the temporary files will be /tmp/hello.s0, /tmp/hello.s1, and /tmp/hello.cfg

X. Further information

You may copy and distribute this program freely as well as modify it for your purposes but you may NOT distribute hacked copies. Instead send all constructive comments to the me and I (bib) will try to incorporate them into future releases (if any). Your work will be properly credited. Also see the disclaimer in the beginning of this document. To request your own copy send Email to:

boyan@tmnxt1.iit.edu
boyaboy@karl.iit.edu
boyaboy@iitvax (Bitnet)

or contact

Boyan Boyanov
Department of Physics
Illinois Institute of Technology
Chicago,IL 60616 USA

phone (312) 567−3398
fax (312) 567−3396

This is the only way you are sure to have the latest (and hopefully the least buggy) version of the program as well as any future upgrades.

Please direct all bug reports, suggestions for improvements, and requests for further assistance (preferably via Email) to the above addresses. Do not be afraid to complain. The program satisfies my own needs in its present form and unless I receive substantial feedback I will make no effort to change/improve anything.

XI. Acknowledgments

Some parts of this program as well as this document itself have drawn heavily from URGENT (R. Walker and B. Diviacco) and its supporting documentation. The author is greatly indebted to R. Walker (Synchrotrone Trieste) for kindly giving his permission for this. Thanks are due to Pathikrit Bandyopadhyay for thoroughly abusing the code :−). The development of this program was supported in part by a gift from Amoco Corporation.

To those of you who had the patience to read through this entire piece of crap − thank you. Let me know if it was worth the effort.

APPENDIX A. Program diagnostics

Several diagnostic files are provided with the program:

- testbf.txt − sample b−field configuration
- txt2u.f − program to convert taper33.txt into binary format
- yaup.inp − sample input file
- yaup−0.out − output generated with yaup.inp and testbf.txt

To perform program diagnostics:

1) Compile txt2u.f. The same precautions should be used when compiling TXT2U as when compiling yaup, i.e. use static allocation, fold all variables to lower/upper case, and do not optimize.

2) Run txt2u with the following input:

```
_____________________________________________________
txt2u − convert text b−field files to YAUP format.

Input file name ? testbf.txt
Output file name ? test.bf
Magnet period (cm) ? 3.3
```

```
Number of periods ? 75
Number of points per period ? 40

Working...
Done.
```

TXT2U should create a b-field file called test.bf

3) Run YAUP with the provided YAUP.INP. This should produce the following output on your screen

---

```
YAUP 1.3.1 - Yet Another (Useless) Undulator Program
Last modified on APR-13-94
Send bug reports to boyan@tmnxt1.iit.edu
```

```
Reading B-field distribution (in tesla) from file test.bf
Writing output to yaup-0.out
```

```
Beginning calculation of electron trajectory as a function
of the longitudinal  coordinate. The total undulator length
is  247.5 centimeters.

    Pass #     z(m)     % done        error (cm)
      3       2.474     100.0        2.249587E-03

Trajectory calculations completed.
Error after the final pass (cm) :   -7.657119E-11 ( 0.00 % )
Initial betax                   :    9.092205E-05
Final   betax                   :    7.673175E-05
```

```
Beginning zero-emittance brightness calculations.
emin =   7000.0   emax =  10000.0   ne = 201
xmin =   -.0480   xmax =   0.0000   nx =  30
ymin =   -.0180   ymax =   0.0000   ny =  12

   x (mrad/mm)  y (mrad/mm)  % done
     0.0000       0.0000      100.0
```

```
Convoluting with the beam divergence.

energy (eV)            % done
    10000.              100
```

This calculation takes about 10 minutes on a 25 MHz 68040 NeXTStation. If the output file (e.g. YAUP-1.OUT) does not reproduce the provided YAUP-0.OUT with sufficient accuracy (1-2 % at the very least) you may need to make some adjustments. Send DETAILED email to boyan@tmnxt1.iit.edu, and I will try to help you solve the problem.

APPENDIX B. Error messages.

Some nice day when I have nothing better to do I'll describe all error messages here. Don't count on it though :-).

07/94 Chicago bib