How to select nonlinear crystals and model their performance using SNLO software

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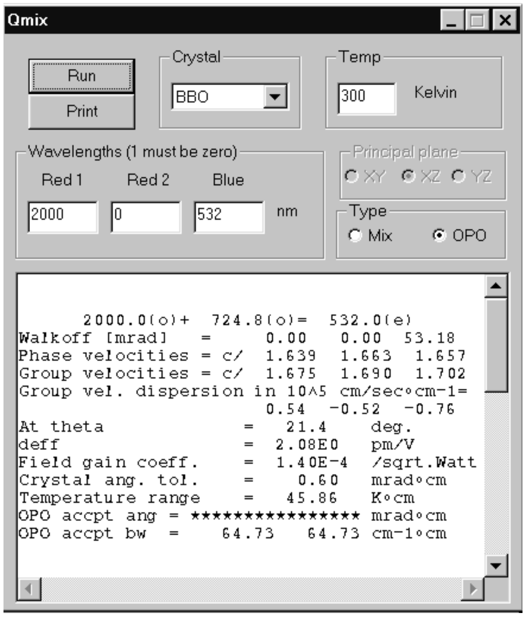
ABSTRACT

SNLO is public domain software developed at Sandia Nat. Labs. It is intended to assist in the selection of the best nonlinear crystal for a particular application, and in predicting its performance. This paper briefly describes its functions and how to use them. Keywords: optical parametric mixing, optical parametric oscillator, nonlinear crystals, nonlinear optics software

1. INTRODUCTION

The advent of powerful desktop computers has made it possible to automate calculations of the linear and nonlinear properties of crystals, and to perform detailed simulations of nonlinear mixing processes in crystals. The purpose of SNLO is to make these calculations available to the public in a free, user-friendly, windows-based package, with the hope that this will advance the state of the art in applications such as optical parametric oscillators/amplifiers (OPO/OPA), optical parametric generation (OPG), frequency doublers, etc. There are three types of functions included in the SNLO menu, shown to the right. The first set help in computing the crystal properties such as phase-matching angles, effective nonlinear coefficients, group velocity, and birefringence. They include functions <u>Ref. Ind.</u>, <u>Qmix</u>, <u>Bmix</u>, <u>QPM</u>, <u>Opoangles</u>, and <u>GVM</u>. The second set, functions <u>PW-mix-LP</u>, <u>PW-mix-SP</u>, <u>PW-mix-BB</u>, <u>2D-mix-LP</u>, <u>2D-mix-SP</u>, <u>PW-OPO-LP</u>, <u>PW-OPO-SP</u>, <u>PW-OPO-BB</u>, and <u>2D-OPO-LP,</u> model the performance of nonlinear crystals in various applications, and the third set, <u>Focus</u>, <u>Cavity</u>, and <u>Help</u>, are helper functions for designing stable cavities, computing gaussian focus parameters, and displaying help text for each of the functions. The capabilities of select functions are presented below.

2. CRYSTAL PROPERTY CALCULATIONS



Crystal: BBO
Temp: 300 Kelvin
Wavelengths (1 must be zero): Red 1 2000, Red 2 0, Blue 532 nm
Type: ○ Mix ● OPO

```
      2000.0(o)+  724.8(o)=  532.0(e)
Walkoff [mrad]   =      0.00   0.00  53.18
Phase velocities = c/  1.639  1.663  1.657
Group velocities = c/  1.675  1.690  1.702
Group vel. dispersion in 10^5 cm/sec∘cm-1=
                       0.54  -0.52  -0.76
At theta              =   21.4     deg.
deff                  =  2.08E0    pm/V
Field gain coeff.     =  1.40E-4   /sqrt.Watt
Crystal ang. tol.     =    0.60    mrad∘cm
Temperature range     =   45.86    K∘cm
OPO accpt ang = **************** mrad∘cm
OPO accpt bw  =    64.73   64.73 cm-1∘cm
```

2.1 Selecting angle-tuned crystals

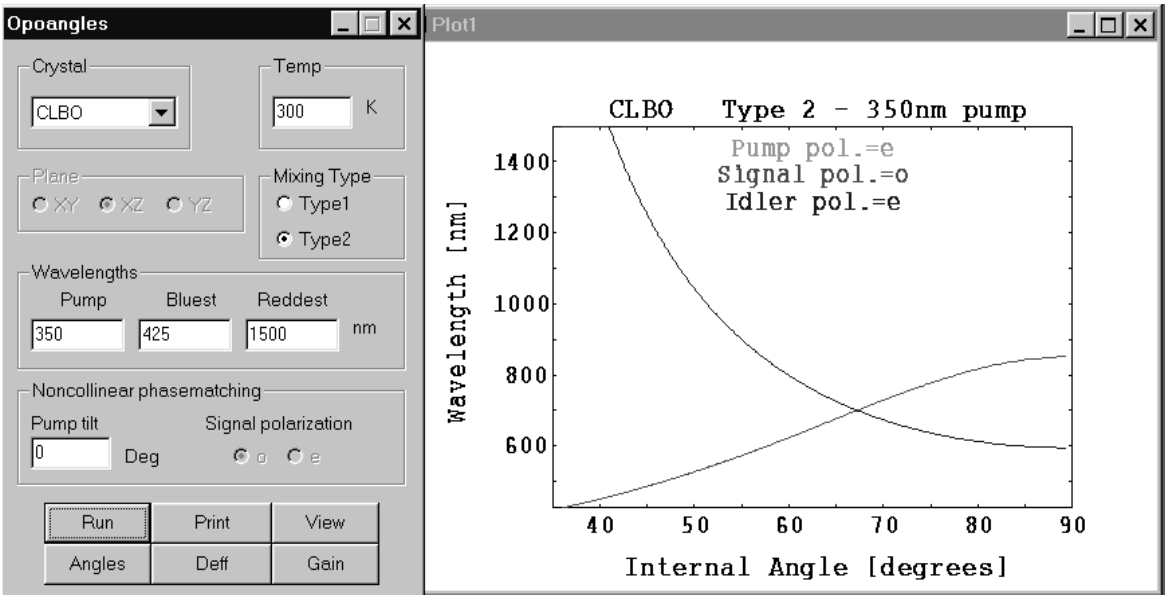
The function <u>QMIX</u> is the best starting place for selecting a nonlinear crystal for your application. When you select a crystal from the list of 40+ crystals, the viewing area will display its properties, including the transmission range (as a plot if the information is available), references for Sellmeier data, nonlinear coefficients, damage thresholds, etc. Enter the wavelengths for your mixing process and push the 'Run' button to compute information specific to all possible phase-matched processes for the selected crystal at the specified wavelengths. The figure to the left shows one example. Note that for biaxial crystals only the principal planes are allowed in <u>QMIX</u>. If you are curious about a biaxial crystal's properties outside the principal planes, you can explore them using <u>BMIX</u>. Further information on crystal properties is available in the papers listed in the bibliography 'Crystals.pdf' included with SNLO. It references over 600 papers relating to nonlinear optical crystals.

2.2 Selecting quasiphase-matched crystals

The function QPM helps you find the right quasiphase matched poling period for any of the popular quasiphase matchable crystals. It also computes temperature and pump wavelength tuning properties for the crystal. You can chose the polarizations for your processes as well, although the *zzz* polarization is usually the one of practical interest.

2.3 Selecting angle-tuned OPO crystals

As shown below, the function Opoangles displays a plot of the signal/idler wavelength versus crystal angle for a given pump wavelength. It also computes the nonlinear coefficient and the parametric gain versus angle. Comparing gain over the wavelength range of interest between different crystals and phase matching types gives a good indication of relative OPO performance. Note that this function permits noncollinear phase matching. Clicking on the ‘pump tilt’ edit box displays a diagram of the noncollinear angles. The signal is assumed to remain aligned to the cavity of an OPO, the pump is tilted by a fixed angle relative to the signal while the crystal and idler tilt by variable amounts to achieve phase match.



Opoangles

Crystal: CLBO

Temp: 300 K

Plane: ○ XY ● XZ ○ YZ

Mixing Type: ○ Type1 ● Type2

Wavelengths: Pump 350, Bluest 425, Reddest 1500 nm

Noncollinear phasematching: Pump tilt 0 Deg; Signal polarization ● o ○ e

2.4 Computing a crystal’s linear optical properties

The function Ref. Ind. can be used to compute refractive indices, group velocities, group velocity dispersions, and birefringent walk off for a given propagation angle, temperature, and wavelength. This is useful if you want to make your own calculations of phase matching, group velocity matching, etc.

2.4 Computing group velocity in angle-tuned crystals

The function GVM computes the phase matching angles and group velocities for noncollinear phase matching. The slant parameter specifies the angle between the pump (bluest) wave’s pulse envelope and its k-vector. All the pulse envelopes are assumed to have the same orientation so if they are all group velocity matched there is no temporal (longitudinal) walk off, but there is spatial (lateral) walk off. For a set of wavelengths and polarizations, the relative group velocities can be varied by changing the value of the slant. In many cases it is possible to achieve perfect group velocity matching in this way. This has obvious application in fs mixing, but it can also be used in mixing broadband light with temporal structure on a fs or ps scale.

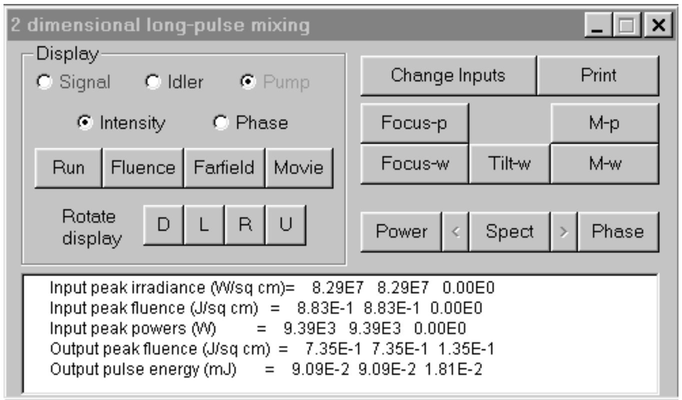
3. NONLINEAR MIXING MODELS

3.1 Modeling single-pass mixing

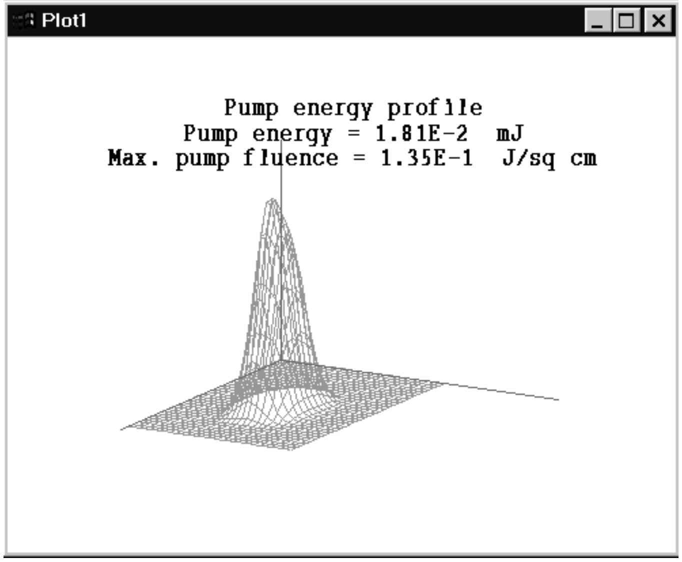
The functions with ‘mix’ in their title handle single-pass mixing, as opposed to mixing in an optical cavity. The functions with the ‘PW’ prefix model plane-wave mixing, those with the ‘2D’ prefix include Gaussian spatial profiles with diffraction and birefringent walk off. The plane-wave models run much faster than the ‘2D’ models, so they can be used to arrive at an approximate set of conditions that can then be fine tuned with the diffractive models.

The functions with suffix ‘LP’ ignore group velocity effects and are appropriate for monochromatic ns and longer pulses, or for monochromatic cw beams. Functions with suffix ‘SP’ incorporate group velocity effects and are useful for ps and fs pulses. The suffix ‘BB’ indicates that the pulses are long but broadband so there is temporal structure on a time scale short enough to require inclusion of group velocity effects.

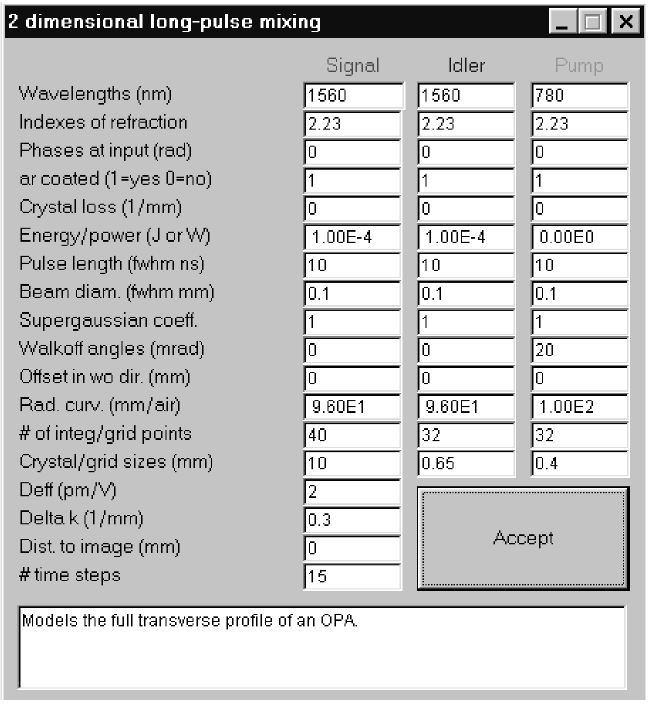
The figure below shows an example of the function 2D-mix-LP. Using the input parameters shown on the input form to the right, it computes near- and far-field spatial fluence profiles as well as spatial profiles and phase profiles as a function of time. Other computed parameters include spectra, power, and beam parameters focus, tilt, and M^2.



```
Input peak irradiance (W/sq cm)=    8.29E7  8.29E7  0.00E0
Input peak fluence (J/sq cm)  =    8.83E-1  8.83E-1  0.00E0
Input peak powers (W)        =    9.39E3  9.39E3  0.00E0
Output peak fluence (J/sq cm) =    7.35E-1  7.35E-1  1.35E-1
Output pulse energy (mJ)      =    9.09E-2  9.09E-2  1.81E-2
```



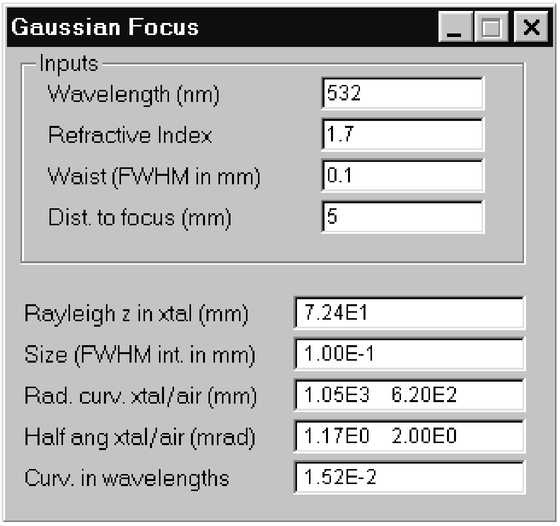
```
Pump energy profile
Pump energy = 1.81E-2  mJ
Max. pump fluence = 1.35E-1  J/sq cm
```



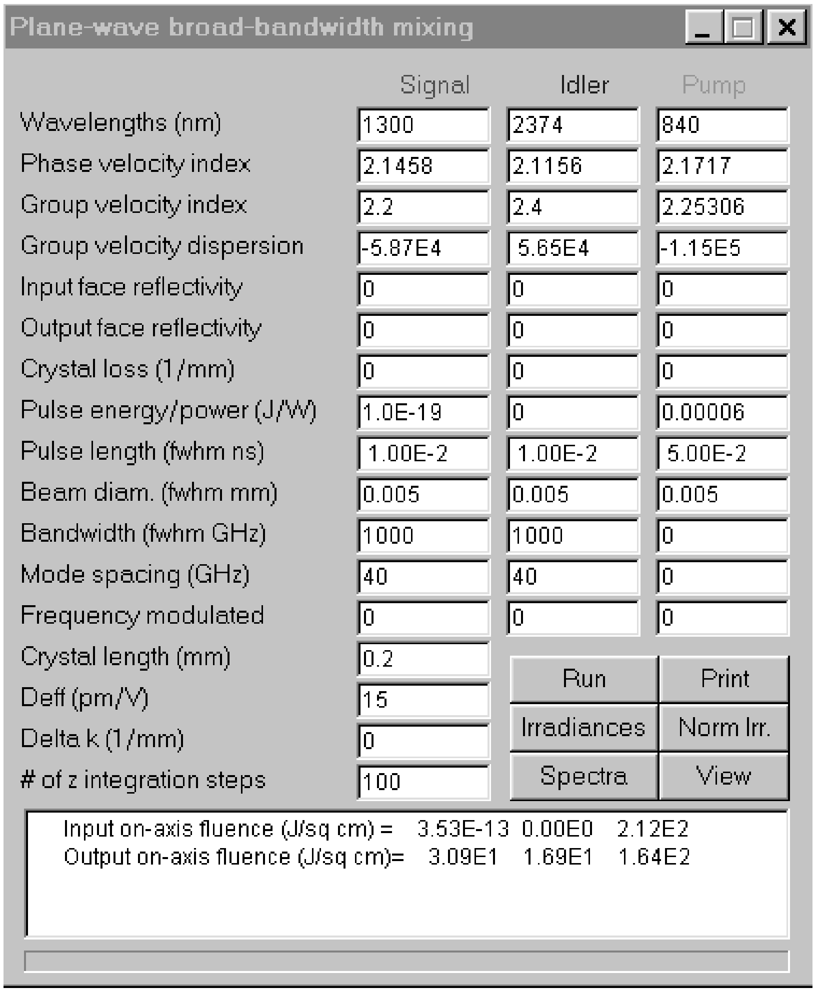
	Signal	Idler	Pump
Wavelengths (nm)	1560	1560	780
Indexes of refraction	2.23	2.23	2.23
Phases at input (rad)	0	0	0
ar coated (1=yes 0=no)	1	1	1
Crystal loss (1/mm)	0	0	0
Energy/power (J or W)	1.00E-4	1.00E-4	0.00E0
Pulse length (fwhm ns)	10	10	10
Beam diam. (fwhm mm)	0.1	0.1	0.1
Supergaussian coeff.	1	1	1
Walkoff angles (mrad)	0	0	20
Offset in wo dir. (mm)	0	0	0
Rad. curv. (mm/air)	9.60E1	9.60E1	1.00E2
# of integ/grid points	40	32	32
Crystal/grid sizes (mm)	10	0.65	0.4
Deff (pm/V)	2		
Delta k (1/mm)	0.3		
Dist. to image (mm)	0		
# time steps	15		

Models the full transverse profile of an OPA.

Usually mixing of low power beams involves focused light, often with a confocal length set comparable to the crystal length. The helper function Focus, shown at the right, is included to help calculate the wavefront curvature at the entrance face of the crystal for such focusing beams. Its output values are automatically updated whenever one of the input parameters is changed.



Wavelength (nm)	532
Refractive Index	1.7
Waist (FWHM in mm)	0.1
Dist. to focus (mm)	5
Rayleigh z in xtal (mm)	7.24E1
Size (FWHM int. in mm)	1.00E-1
Rad. curv. xtal/air (mm)	1.05E3 6.20E2
Half ang xtal/air (mrad)	1.17E0 2.00E0
Curv. in wavelengths	1.52E-2

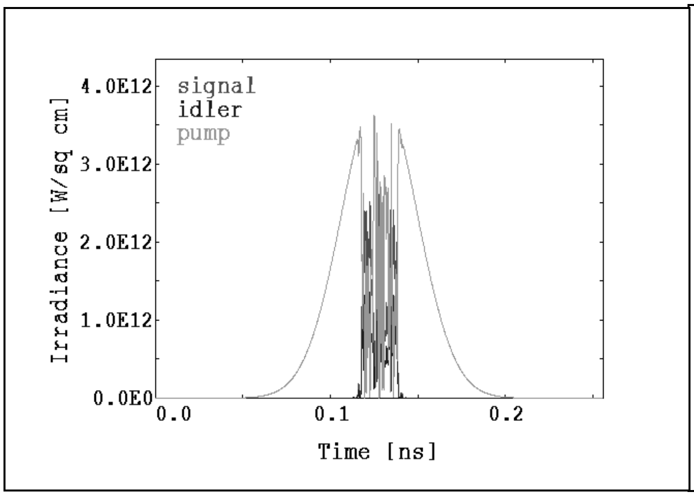


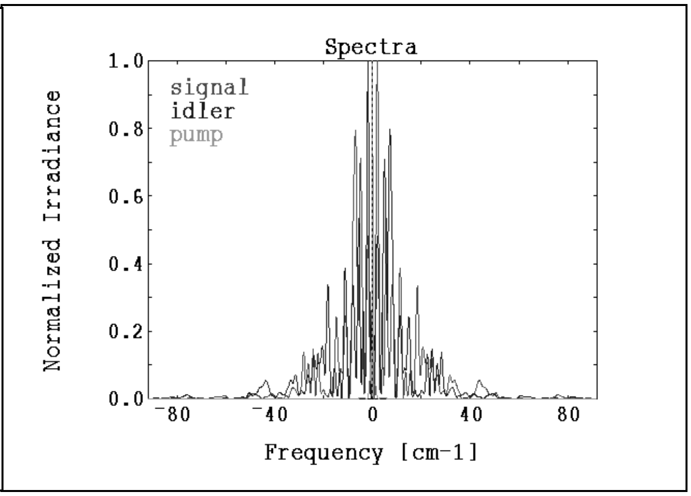
Plane-wave broad-bandwidth mixing

	Signal	Idler	Pump
Wavelengths (nm)	1300	2374	840
Phase velocity index	2.1458	2.1156	2.1717
Group velocity index	2.2	2.4	2.25306
Group velocity dispersion	-5.87E4	5.65E4	-1.15E5
Input face reflectivity	0	0	0
Output face reflectivity	0	0	0
Crystal loss (1/mm)	0	0	0
Pulse energy/power (J/W)	1.0E-19	0	0.00006
Pulse length (fwhm ns)	1.00E-2	1.00E-2	5.00E-2
Beam diam. (fwhm mm)	0.005	0.005	0.005
Bandwidth (fwhm GHz)	1000	1000	0
Mode spacing (GHz)	40	40	0
Frequency modulated	0	0	0
Crystal length (mm)	0.2		
Deff (pm/V)	15		
Delta k (1/mm)	0		
# of z integration steps	100		

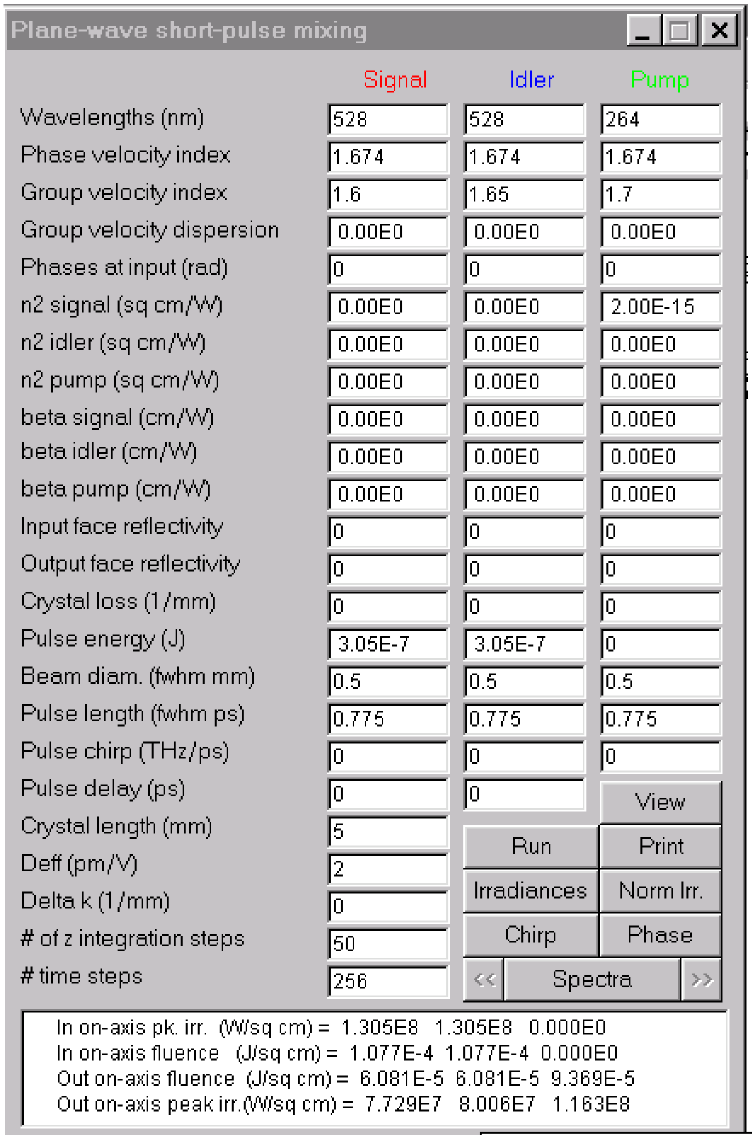
```
Input on-axis fluence (J/sq cm) =   3.53E-13  0.00E0   2.12E2
Output on-axis fluence (J/sq cm)=   3.09E1   1.69E1   1.64E2
```

The function PW-mix-BB can be used to model optical parametric generation (OPG) as a high-gain case of single-pass mixing in the plane-wave approximation. You must specify the correct signal and idler energies, bandwidths, and mode spacings to simulate start-up quantum noise. The mode spacing should be the inverse of the signal/idler pulse length. For example, if you have a 1 ps pump pulse, you could use 5 ps signal and idler pulses (to allow for temporal walk off) and a signal/idler mode spacing of 100 GHz. The bandwidth should be set to several times the OPO acceptance bandwidth, and the pulse energy of the signal and idler should be set so there is one photon per mode, ie energy = hν×bandwidth÷(mode spacing). Because the gain is very high for OPG, the number of *z* integration steps must be quite large. I suggest you start with 100 steps and double it until the results converge. Each run will use different start up noise, so convergence does not mean identical results here. A good test is to look at both the irradiance and spectral plots and make sure they are both similar to the previous run with fewer integration steps. The figures above show an example of an OPG calculation. The parameters are specified in the input form on the left and the output time profile is shown below.



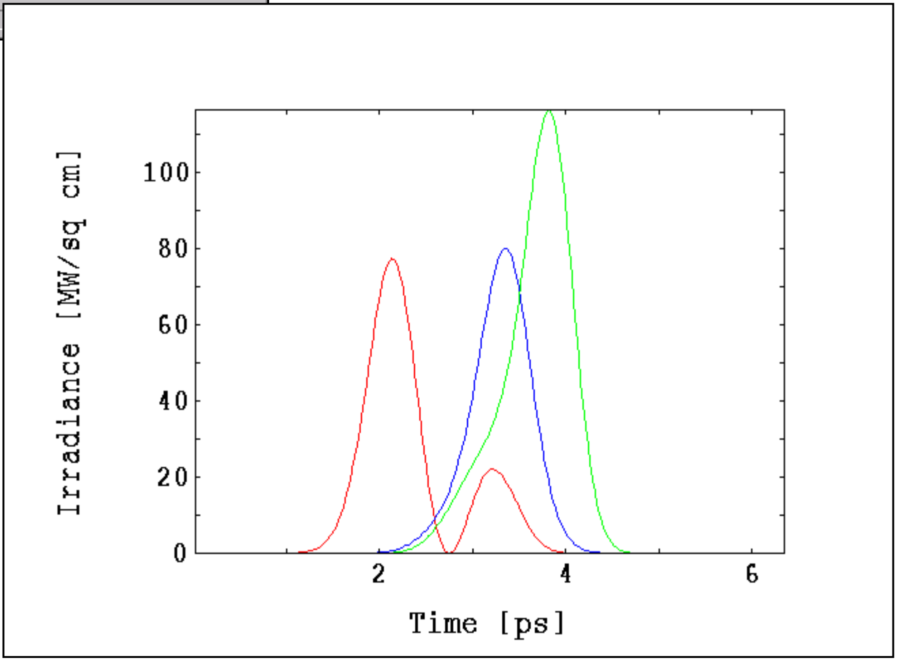


The functions PW-mix-SP and 2D-mix-SP model single pass mixing for pulses short enough that group velocity effects are important. The figure below show an example for the plane-wave case. The signal and idler pulses are given an input energy and the pump pulse is generated in the crystal. The signal and idler pulses separate in time due to group velocity differences and reshape due to group velocity dispersion. The slower pump pulse emerges with a time delay. The "movie" button displays the pulses as they would appear inside the crystal propagating at different velocities and changing strength through nonlinear mixing. In this function as well as most of the other functions, you can specify the energy in any of the pulses, there is no assumption of sum-frequency mixing or optical parametric gain. Mixing will proceed just as in a real crystal. If there are three nonzero inputs, the direction of energy transfer will depend on the relative phase of the three beams.



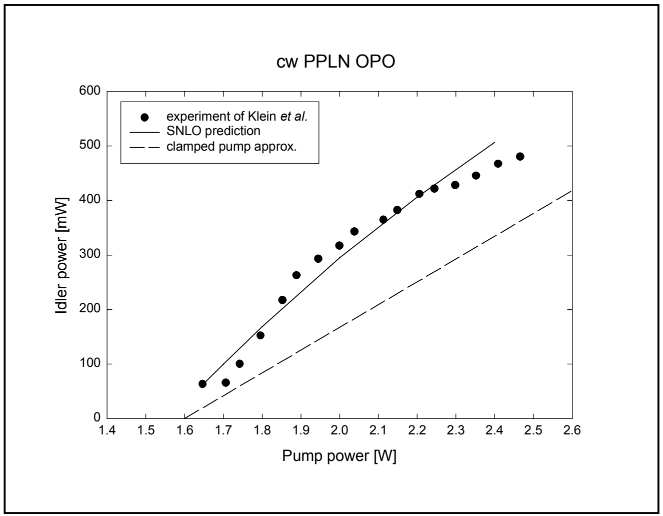
	Signal	Idler	Pump
Wavelengths (nm)	528	528	264
Phase velocity index	1.674	1.674	1.674
Group velocity index	1.6	1.65	1.7
Group velocity dispersion	0.00E0	0.00E0	0.00E0
Phases at input (rad)	0	0	0
n2 signal (sq cm/W)	0.00E0	0.00E0	2.00E-15
n2 idler (sq cm/W)	0.00E0	0.00E0	0.00E0
n2 pump (sq cm/W)	0.00E0	0.00E0	0.00E0
beta signal (cm/W)	0.00E0	0.00E0	0.00E0
beta idler (cm/W)	0.00E0	0.00E0	0.00E0
beta pump (cm/W)	0.00E0	0.00E0	0.00E0
Input face reflectivity	0	0	0
Output face reflectivity	0	0	0
Crystal loss (1/mm)	0	0	0
Pulse energy (J)	3.05E-7	3.05E-7	0
Beam diam. (fwhm mm)	0.5	0.5	0.5
Pulse length (fwhm ps)	0.775	0.775	0.775
Pulse chirp (THz/ps)	0	0	0
Pulse delay (ps)	0	0	
Crystal length (mm)	5		
Deff (pm/V)	2		
Delta k (1/mm)	0		
# of z integration steps	50		
# time steps	256		

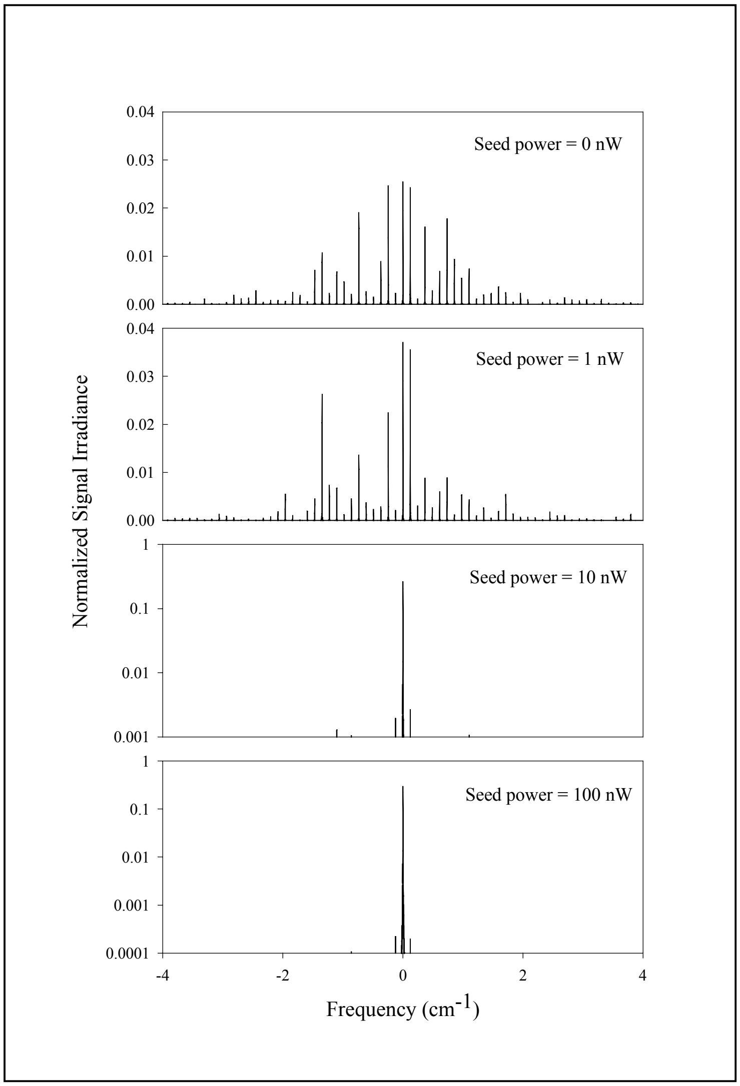
```
In on-axis pk. irr.  (W/sq cm) =  1.305E8   1.305E8   0.000E0
In on-axis fluence   (J/sq cm) =  1.077E-4  1.077E-4  0.000E0
Out on-axis fluence  (J/sq cm) =  6.081E-5  6.081E-5  9.369E-5
Out on-axis peak irr.(W/sq cm) =  7.729E7   8.006E7   1.163E8
```



3.2 Model mixing in a cavity (OPO, frequency doubling, etc.)

The functions with ‘OPO’ in their title can model mixing in a cavity. Note that most of these models will handle not only OPO’s but any mixing process in a cavity, including frequency doubling in a build-up cavity. Functions with the ‘PW’ prefix model plane-wave mixing; those with the ‘2D’ prefix include Gaussian spatial profiles with diffraction and birefringent walk off, and they can accommodate curved cavity mirrors. The functions with suffix ‘LP’ ignore group velocity effects and are intended to model ns and longer pulses or cw beams. As an example of diffractive modeling, the figure to the right compares 2D-OPO-LP modeling of a cw, stable-cavity OPO with experimental measurements by Klein *et al.*[1] The only adjustable input parameter is the round-trip cavity loss which was not precisely measured. For cw cases the model continues to run and display a number indicating the amount of change on the last cavity pass. You terminate the run by pressing the “Stop” button when the convergence is satisfactory. Another example may be found in one of our earlier papers[2] in which we compared the predictions of 2D-OPO-LP with measurements of a pulsed OPO, obtaining excellent agreement between experiment and model, with no adjustable parameters, for a nanosecond, KTP, ring OPO.



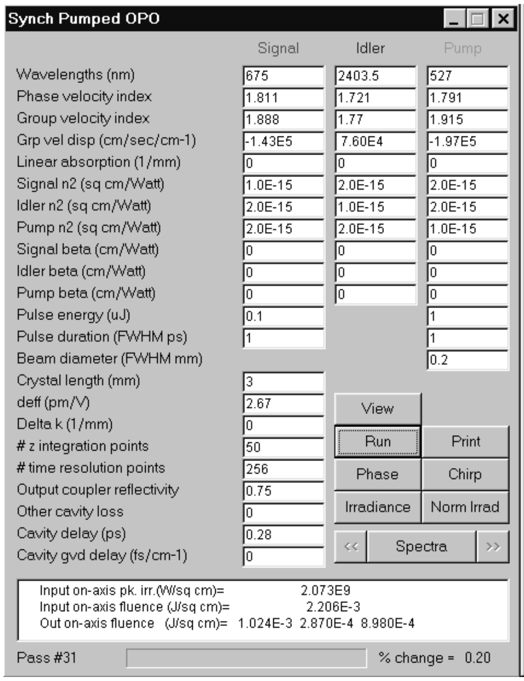


The function with the suffix ‘SP’, PW-OPO-SP, incorporates group velocity effects to model OPO’s synchronously-pumped by ps or fs pulses.

The suffix ‘BB’ indicates that the pulses are of long duration but have a broad bandwidth so there is temporal structure on a time scale short enough to require the inclusion of group velocity effects. The figure at the left demonstrates the use of PW-OPO-BB to study injection seeding of an OPO. The top plot is the signal spectrum of an OPO without seeding. Succeeding plots are the signal spectra with increasing seed power, demonstrating the spectral collapse to a single mode at a seed power of a few nW. Further details are given in ref. 3.

Generally the mixing of low power beams is done in a stable cavity formed by focusing mirrrors. Such cavities can be designed using the Cavity function which will also help you find the wavefront curvature of the input beams at the input mirror, and the cavity round-trip phase which must be known to achieve exact resonance in the cavity. This function operates much like Focus in that the outputs are updated automatically on any change of the input parameters. A help plot of the cavity pops up with this function to assist in setting the parameters.

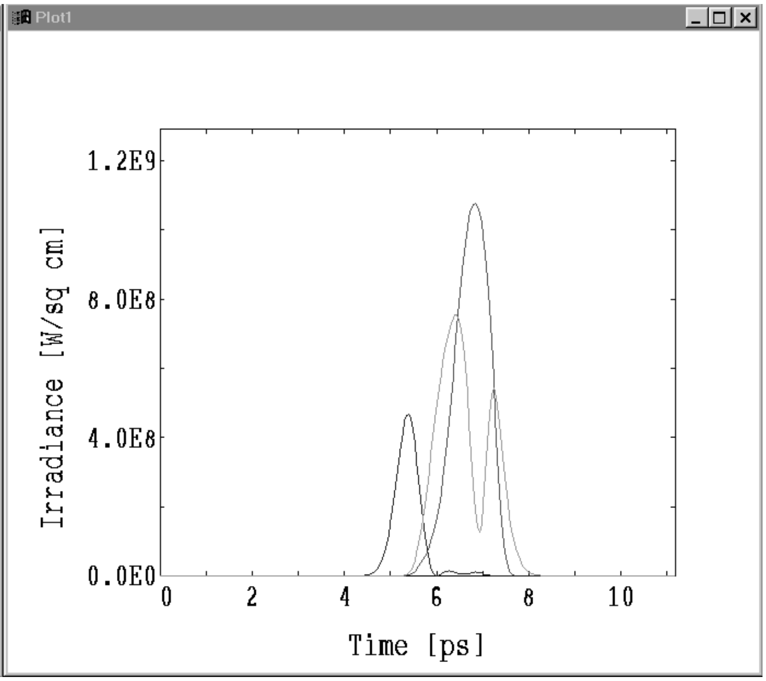
The function PW-OPO-SP, unlike the other cavity mixing functions, is limited to OPO modeling, and will not handle general cavity mixing. More specifically it is limited to synchronously pumped OPO's. The cavity is assumed to be a singly-resonant ring as diagrammed on the left, with a nonlinear crystal in one leg and a group velocity dispersion compensator in the another leg. A sample input form and resulting output pulses are shown below. Like other cw modeling, this function runs until you are satisfied with the convergence of the output and terminate the run.



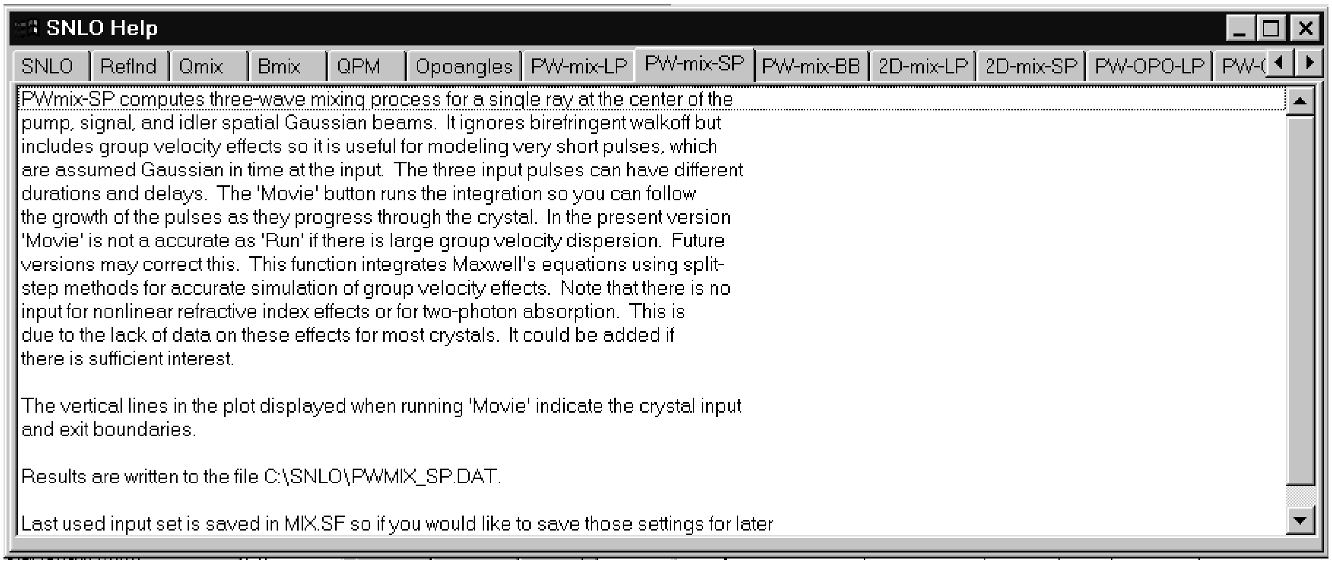
	Signal	Idler	Pump
Wavelengths (nm)	675	2403.5	527
Phase velocity index	1.811	1.721	1.791
Group velocity index	1.888	1.77	1.915
Grp vel disp (cm/sec/cm-1)	-1.43E5	7.60E4	-1.97E5
Linear absorption (1/mm)	0	0	0
Signal n2 (sq cm/Watt)	1.0E-15	2.0E-15	2.0E-15
Idler n2 (sq cm/Watt)	2.0E-15	1.0E-15	2.0E-15
Pump n2 (sq cm/Watt)	2.0E-15	2.0E-15	1.0E-15
Signal beta (cm/Watt)	0	0	0
Idler beta (cm/Watt)	0	0	0
Pump beta (cm/Watt)	0	0	0
Pulse energy (uJ)	0.1		1
Pulse duration (FWHM ps)	1		1
Beam diameter (FWHM mm)			0.2
Crystal length (mm)	3		
deff (pm/V)	2.67		
Delta k (1/mm)	0		
# z integration points	50		
# time resolution points	256		
Output coupler reflectivity	0.75		
Other cavity loss	0		
Cavity delay (ps)	0.28		
Cavity gvd delay (fs/cm-1)	0		

```
Input on-axis pk. irr.(W/sq cm)=              2.073E9
Input on-axis fluence (J/sq cm)=               2.206E-3
Out on-axis fluence   (J/sq cm)=  1.024E-3  2.870E-4  8.980E-4
```

Pass #31 % change = 0.20



The Help function offers a short description of each function along with hints on its use and a list of the output files written by each. One example is displayed here.



PWmix-SP computes three-wave mixing process for a single ray at the center of the pump, signal, and idler spatial Gaussian beams. It ignores birefringent walkoff but includes group velocity effects so it is useful for modeling very short pulses, which are assumed Gaussian in time at the input. The three input pulses can have different durations and delays. The 'Movie' button runs the integration so you can follow the growth of the pulses as they progress through the crystal. In the present version 'Movie' is not a accurate as 'Run' if there is large group velocity dispersion. Future versions may correct this. This function integrates Maxwell's equations using split-step methods for accurate simulation of group velocity effects. Note that there is no input for nonlinear refractive index effects or for two-photon absorption. This is due to the lack of data on these effects for most crystals. It could be added if there is sufficient interest.

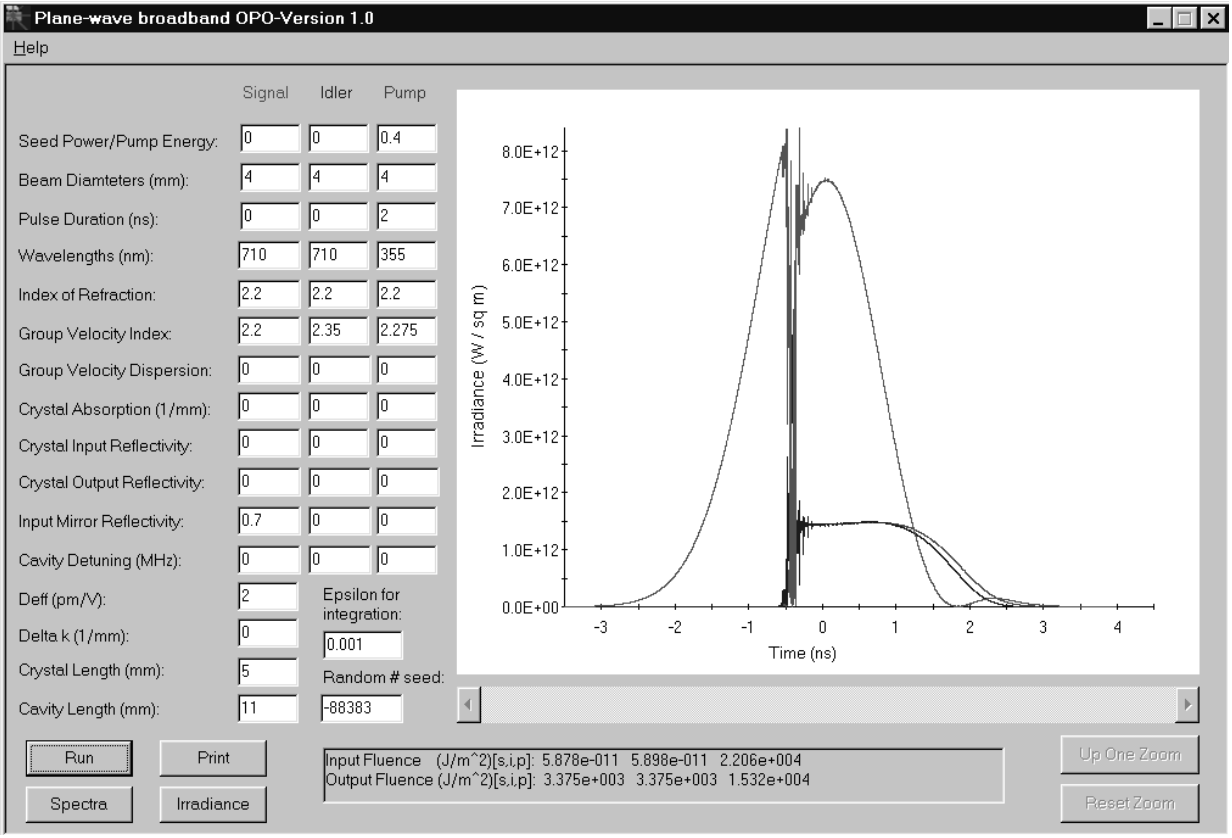
The vertical lines in the plot displayed when running 'Movie' indicate the crystal input and exit boundaries.

Results are written to the file C:\SNLO\PWMIX_SP.DAT.

Last used input set is saved in MIX.SF so if you would like to save those settings for later

4. CONCLUSION

All of the modeling functions of SNLO are based on split-step integration methods. They are state-of-the-art in technique, and are all-numerical to cover the widest possible range of applications. More detail is available in the papers of refs. 2-4. I have carefully validated them against analytical expressions and against each other. SNLO is public domain software written in APL programming language. It may be downloaded free of charge at web site http://www.sandia.gov/imrl/XWEB1128/xxtal.htm . We are translating some of the modeling functions of SNLO as well as additional related modeling functions into C++. They are also public domain and will be posted at the same web address as they become available. Only the function PWOPOBB, show here, is currently available. This function is nearly identical in function to the SNLO function PW-OPO-BB.



	Signal	Idler	Pump
Seed Power/Pump Energy:	0	0	0.4
Beam Diamteters (mm):	4	4	4
Pulse Duration (ns):	0	0	2
Wavelengths (nm):	710	710	355
Index of Refraction:	2.2	2.2	2.2
Group Velocity Index:	2.2	2.35	2.275
Group Velocity Dispersion:	0	0	0
Crystal Absorption (1/mm):	0	0	0
Crystal Input Reflectivity:	0	0	0
Crystal Output Reflectivity:	0	0	0
Input Mirror Reflectivity:	0.7	0	0
Cavity Detuning (MHz):	0	0	0

Deff (pm/V): 2
Delta k (1/mm): 0
Crystal Length (mm): 5
Cavity Length (mm): 11
Epsilon for integration: 0.001
Random # seed: -88383

```
Input Fluence  (J/m^2)[s,i,p]: 5.878e-011  5.898e-011  2.206e+004
Output Fluence (J/m^2)[s,i,p]: 3.375e+003  3.375e+003  1.532e+004
```

Acknowledgement
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

References

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