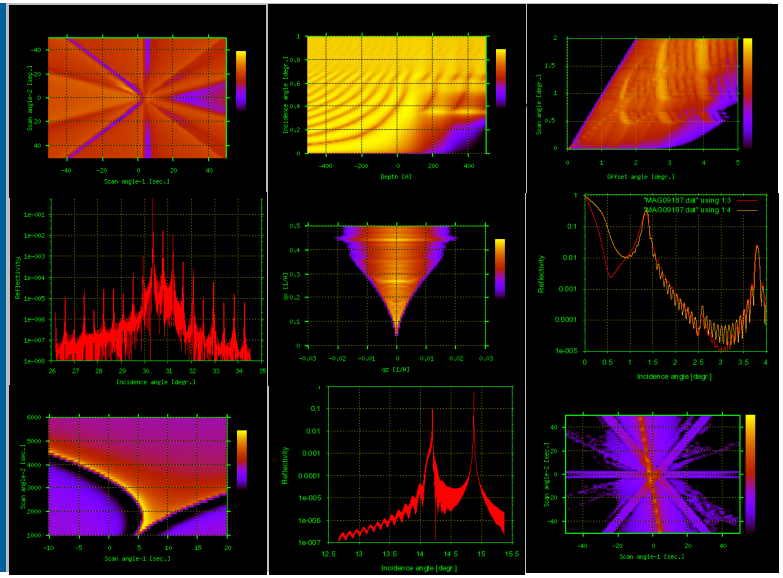
X-RAY SERVER: 28 YEARS ONLINE. LATEST AI-ASSISTED DEVELOPMENTS



SERGEY STEPANOV

Argonne National Laboratory,
Advanced Photon Source,
Lemont, IL, USA

DESY Photon Science Users' Meeting "Research with Synchrotron Radiation and FELs"
January 29, 2026: “Enhancing UX in X-ray Optics: Simulations including AI-driven Applications”

What is X-ray Server?

Let us ask Google Gemini AI: “what is Stepanov X-ray server?”

AI Overview

The Stepanov X-ray Server (x-server.gmca.aps.anl.gov) is a widely used web-based platform for X-ray diffraction and scattering simulations, providing researchers with free access to advanced computational tools developed by X-ray physicist Sergey Stepanov, allowing them to model complex phenomena like dynamical diffraction from crystals and multilayers directly online without software installation. It serves as a vital resource for planning experiments, analyzing data, and fostering scientific collaboration by offering immediate access to sophisticated X-ray modeling software.

Advanced Models: Implements complex physical models for interface roughness, X-ray standing waves, and more.

Established Resource: Online since 1997, it has processed millions of requests, making it a reputable tool in the X-ray community.

Why It's Important

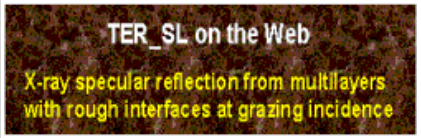
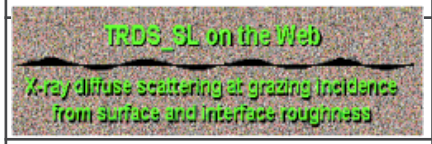
Ease of Use: Provides immediate access to powerful tools, accelerating research.

Collaboration: Facilitates remote collaboration and feedback, helping refine models and software.

Accessibility: Makes advanced X-ray modeling accessible to a broad scientific audience

Software available through X-ray Server

https://x-server.gmca.aps.anl.gov (online since 1997; performed 5,694,899 calculations)

 	***X0h*** interpolates dielectric susceptibilities for crystals and other materials in wide range of X-ray energies with the option to compare data from different DBs. ***X0h+*** provides search for Bragg planes in crystals under various conditions (Bragg angle, strong reflections…).	**3,220,539** **56.6%**
	***GID_sl*** models X-ray diffraction from strained crystals and multilayers for any Bragg-case geometry including grazing incidence/exit and scans around arbitrary axes	**1,947,002** **34.2%**
	***TER_sl*** calculates X-ray specular reflection and respective X-ray standing waves from multilayers with interface roughness and transition layers .	**426,118** **7.5%**
	***BRL*** models multiple Bragg diffraction of X-rays from perfect crystals including the cases of X-rays grazing along the surface and Bragg angles close to 90°.	**56,301** **1.0%**
	***TRDS_sl*** calculates X-ray diffuse scattering for several models of interface roughness in multilayers.	**25,297** **0.4%**
	***MAG_sl*** calculates X-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers.	**19,642** **0.3%**

Based on 19 x-ray research papers. Statistics as of January 19, 2026.

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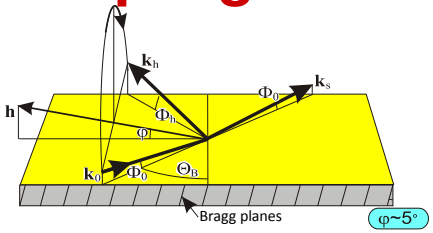
X-ray Server programs

GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

34.2%

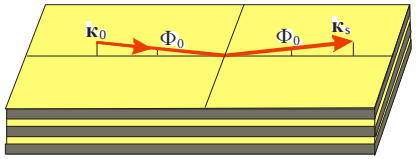


Any Bragg-case diffraction incl. grazing incidence and/or exit

- Calculates Bragg diffraction from crystals with given profiles of normal lattice strains da(z)/a, dielectric susceptibilities $\chi_0(z)$, $\chi_h(z)$, and interface roughness height σ(z). The profiles are specified layer-by-layer, which allows for flexibility.
- Can calculate X-ray standing waves

TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence

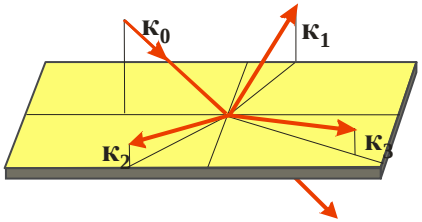
7.5%



- Calculates X-ray specular reflection from plain mirrors and multilayers with given profiles of $\chi_0(z)$ and interface roughness height σ(z) or transition layers.
- Converges faster than the Parratt recursive technique
- Can calculate X-ray standing waves in multilayers

BRL on the Web
X-ray multiple Bragg/Laue diffraction

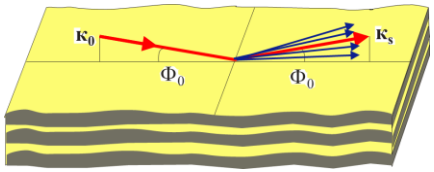
1.0%



- Calculates multiple Bragg diffraction from perfect crystals including X-rays grazing along the surface and Bragg angles close to 90°
- Takes into account specular reflection and refraction of X-rays at crystal surface for grazing X-rays, but neglects for non-grazing.

TRDS_SL on the Web
X-ray diffuse scattering at grazing incidence from surface and interface roughness

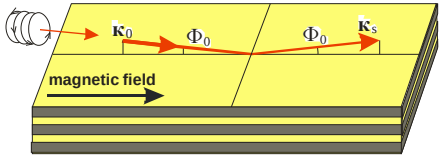
0.4%



- Calculates X-ray diffuse scattering from interface roughness in multilayers
- Implements modeling for 10 different types of roughness correlations between the layers.

MAG_SL on the Web
X-ray resonant specular reflection from magnetic multilayers

0.3%



Calculates resonant X-ray reflectivity from magnetic multilayers

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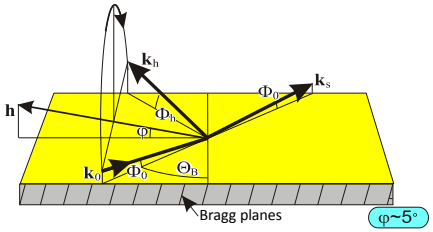
X-ray Server structure factors (X0h)

GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

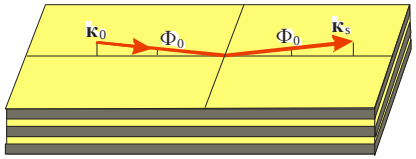
34.2%



Any Bragg-case diffraction incl. grazing incidence and/or exit

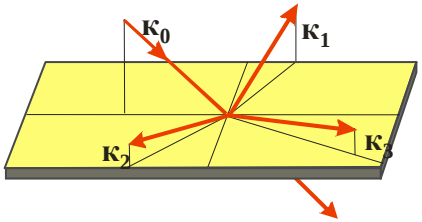
TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence

7.5%



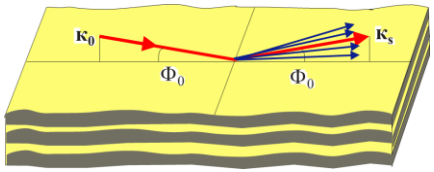
BRL on the Web
X-ray multiple Bragg/Laue diffraction

1.0%



TDS_SL on the Web
X-ray diffuse scattering at grazing incidence from surface and interface roughness

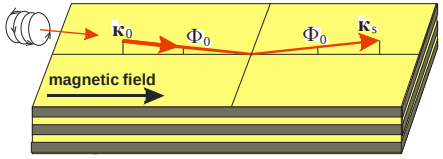
0.4%



circularly polarized X-rays

MAG_SL on the Web
X-ray resonant specular reflection from magnetic multilayers

0.3%



χ_{ot} on the Web !!!

56.6%

- Besides the web interface, also provides X-ray scattering factors for **all** X-ray Server programs.
- Interpolates data from five different tables with option to compare.
- Provides search for Bragg planes under various conditions

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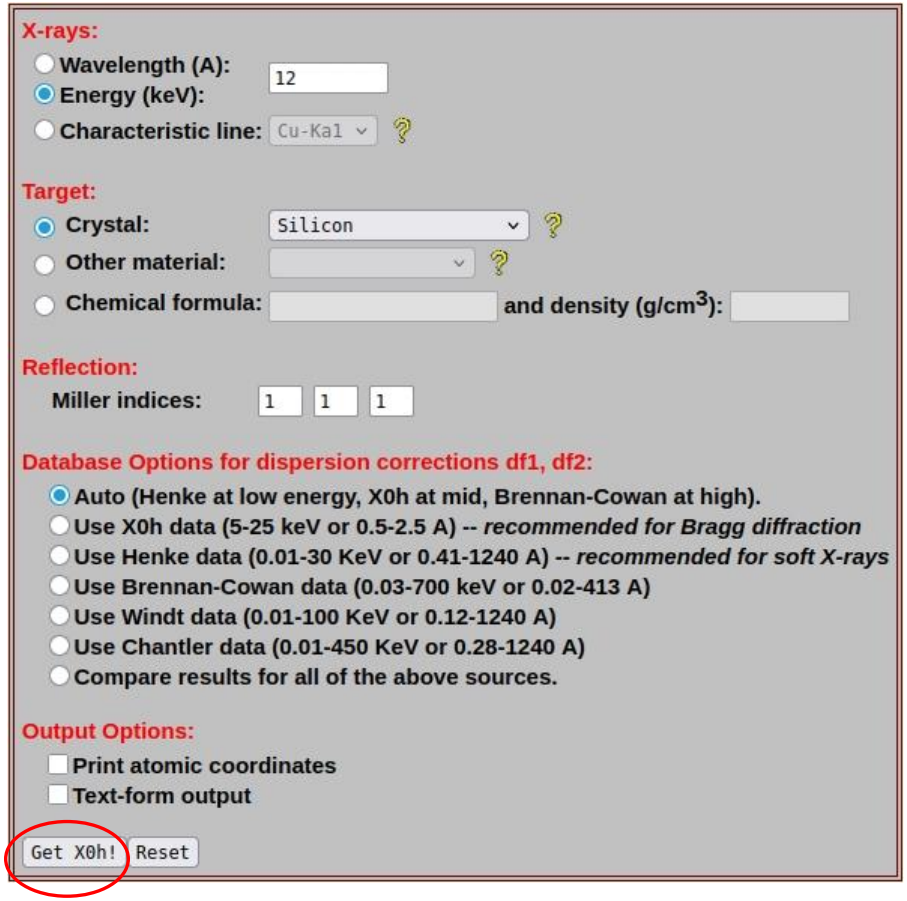
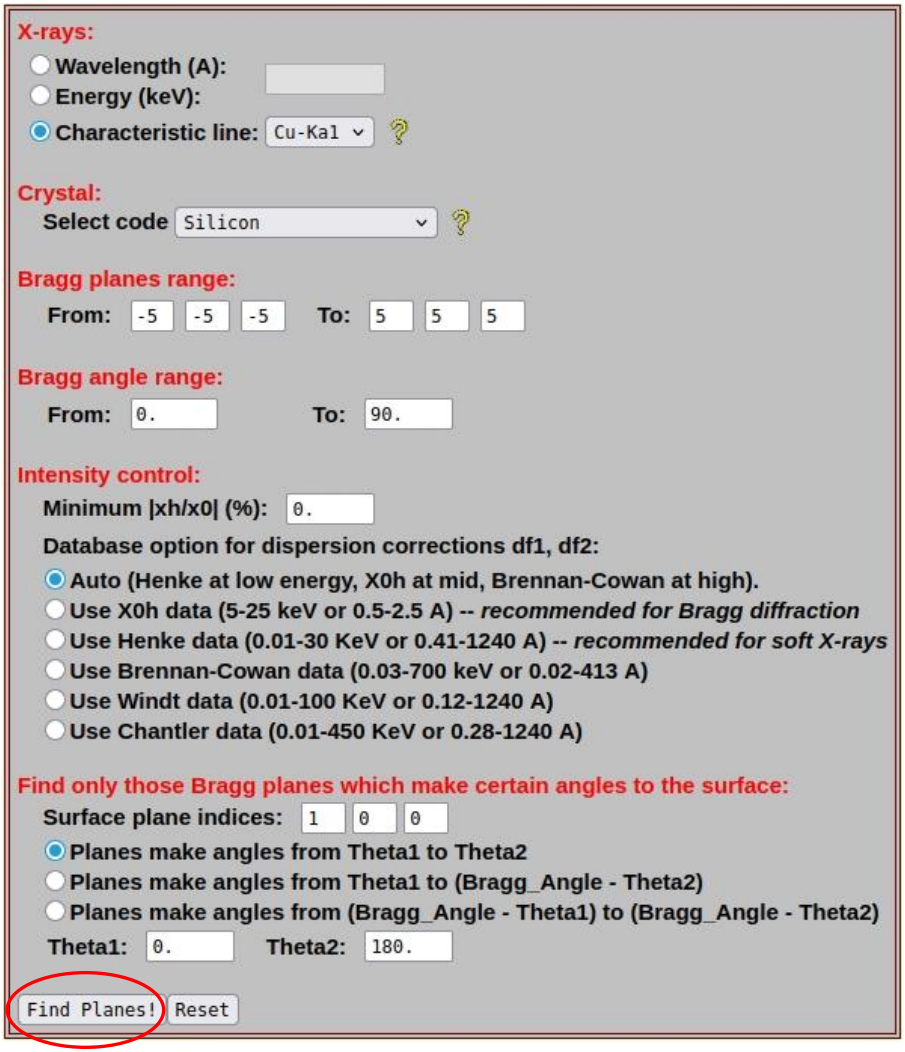
Structure factors: web interfaces





These are not quantum calculations of structure factors, but interpolation of data from publicly available tables of atom properties combined with integration over crystal unit cell

The X0h structures DB currently contains 184 crystals. Most are submitted by users.

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X0h structure submission interface

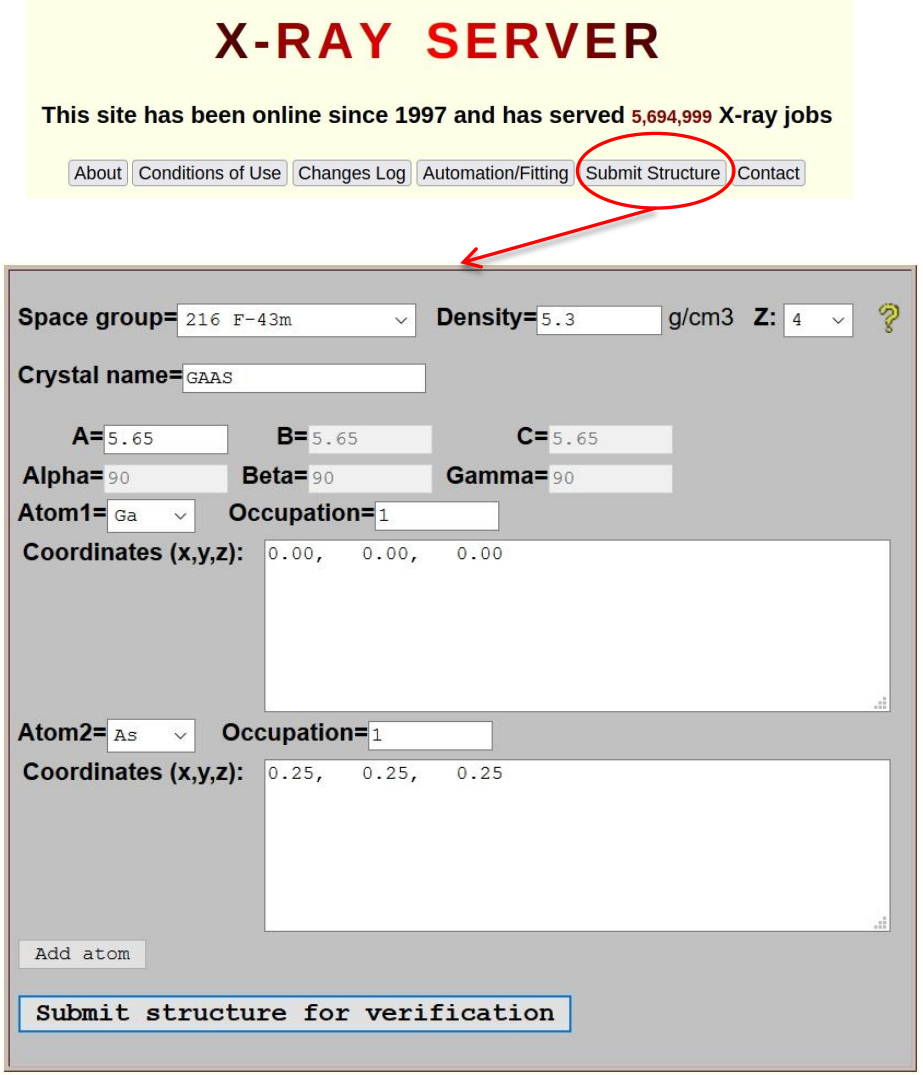
Submission is currently semi-automated: user fills web form which applies space group transformations and makes several checks for consistency. Then, it is sent for further manual inspection and approval.

The reasons for manual checks:

- **Users are not crystallographers and mistakes are frequent.**
- **Once the submitted structure become public, errors put the server, not the submitter reputation at stake.**

Further automation plans:

- Assign temp access code or use submitter's IP address to make the submitted structure available to the submitter only until manual inspection is completed and the structure is made public.



Diffraction program GID_sl web interface

GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

X-rays specified by: Wavelength (A) Value= 1.540562 Line= Cu-Ka1 Polarization= Sigma

Crystal: Germanium Auto DB for f',f" Sigma= 0. A W0= 1. Wh= 1.

Bragg Reflection: 1 1 1 Substrate da/a= 0.

Geometry specified by: angle of Bragg planes to surface ('+' for g0>gh) , Value: 0. degr.

Scan: from -60. to +60. sec. Scan points: 401 Invert axis: Plot argument: scan angle

Standing waves: Reference interface = 0 (0=surface)
Start offset = 0. Angstrom (down from reference)
End offset = 0. Angstrom (down from reference)
Number of offsets = 1 (max = 401)
Location phase/pi = 0 (0-2, empty for no phase)

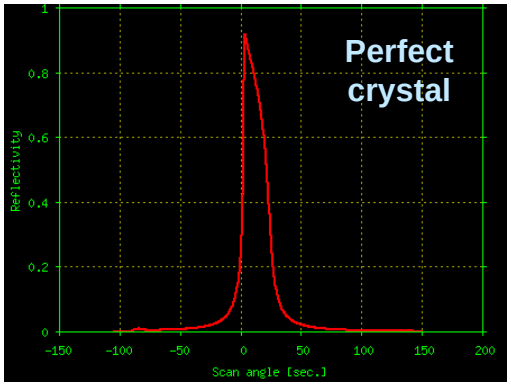
Approximations: alpha_max= 1.E+8 *|xh| **Matrix reduction:** Fly

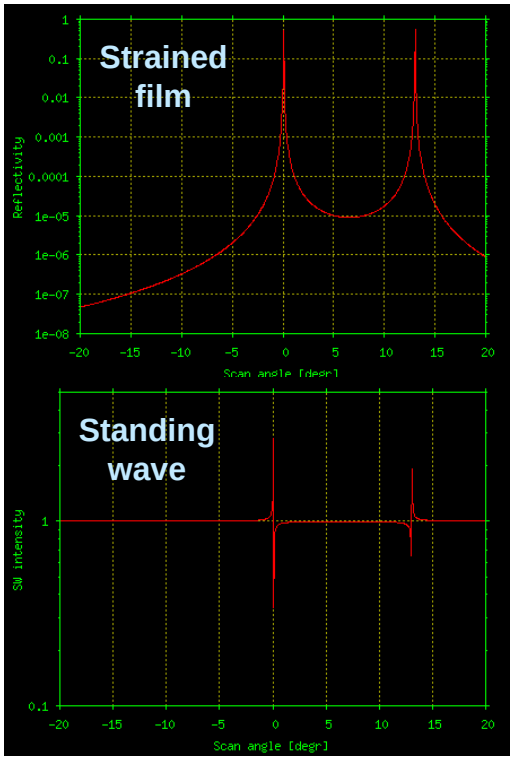
watch progress Submit Query (single click, please!)

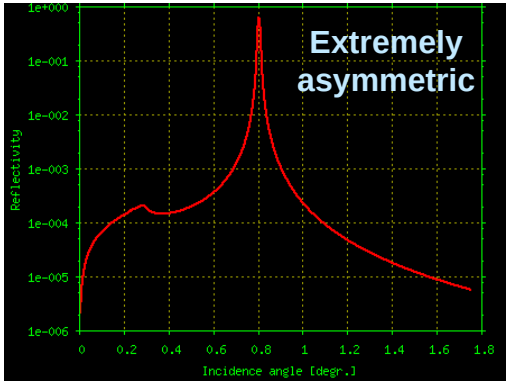
Top layer profile *(optional)*:
period=
t= sigma= da/a= code= x= code2= x2= code3= x3= code4= x0= xh= xhdf= w0= wh= xhphase=
end period

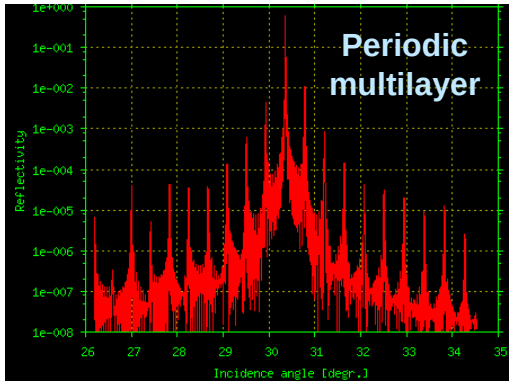
```
period=20
 t=100 code=GaAs sigma=2
 t=70 code=AlAs sigma=2 da/a=a
end period
```

Available codes:
[?] **Crystals:**
ADP
AlAs
AlFe3
AlN
AlP
AlSb









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Reflectivity program TER_sl web interface

TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence

X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line= Cu-Ka1 Polarization= Sigma

Substrate: Database code: GaAs X0h data (5-25keV; 0.5-2.5A)
Chemical formula: rho= g/cm^3
Susceptibility x0 = ( ) / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /
x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /
Roughness: sigma = 4. Angstrom OR Transition layer tr = 0. Angstrom

Incidence angle limits: from 0. to 3. degr. Scan points= 601

Standing waves: Reference interface = 0 (0=surface)
Start offset = 0. Angstrom
End offset = 1000. Angstrom
Number of offsets = 101 (max = 401)

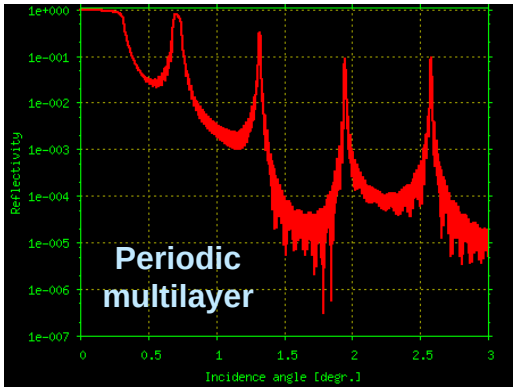
watch progress Submit Query (single click, please!)

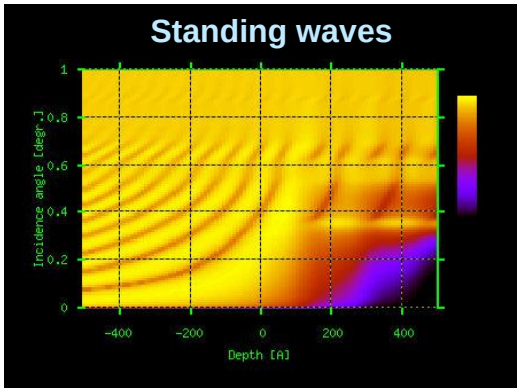
Top layer profile *(optional)*:

```
t=20 w0=0.5 sigma=5   !surface oxide, organic contamination or dust
period=20
t=100 code=GaAs sigma=4
t=70 code=AlAs sigma=4
end period
```

Submit Query (same "Submit" action as above; single click, please!)

Available codes: (use Copy/Paste)
Ac
Ag
Al
Al2O3
AlAs
AlFe3
AlN
AlP





- **Applications**: X-ray optics (mirrors and multilayer mirrors and monochromators) and semiconductor material science
- **Limitations**: no curved mirrors

Plans:
- Add energy scans.

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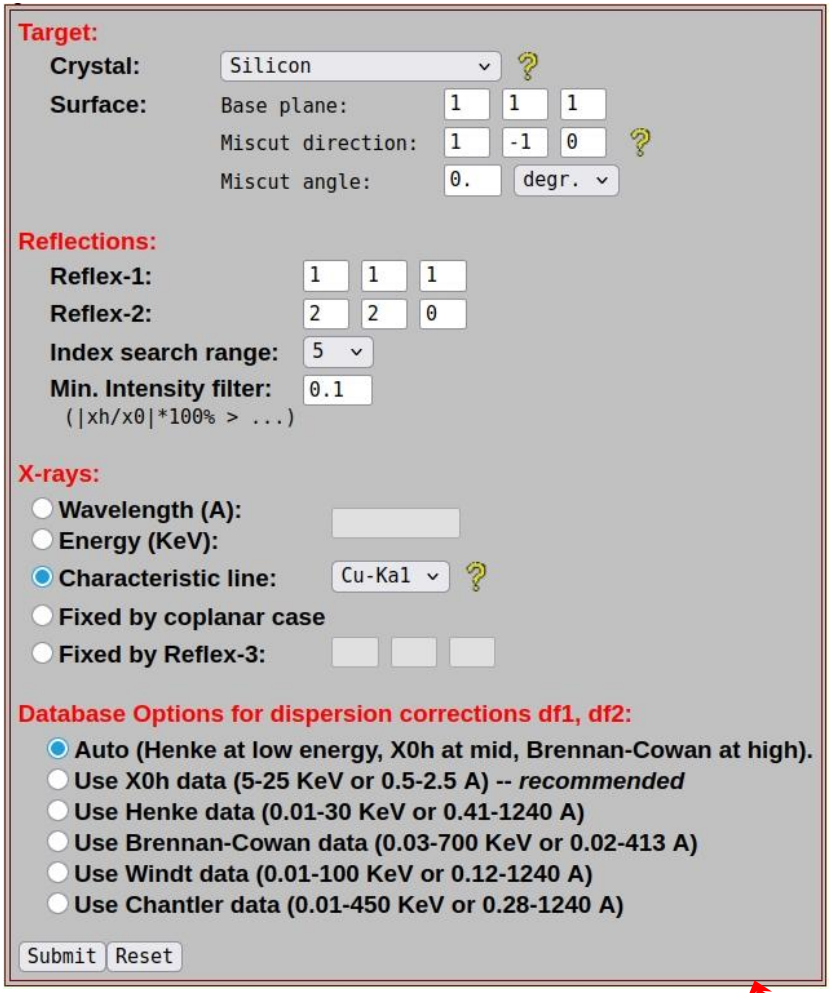
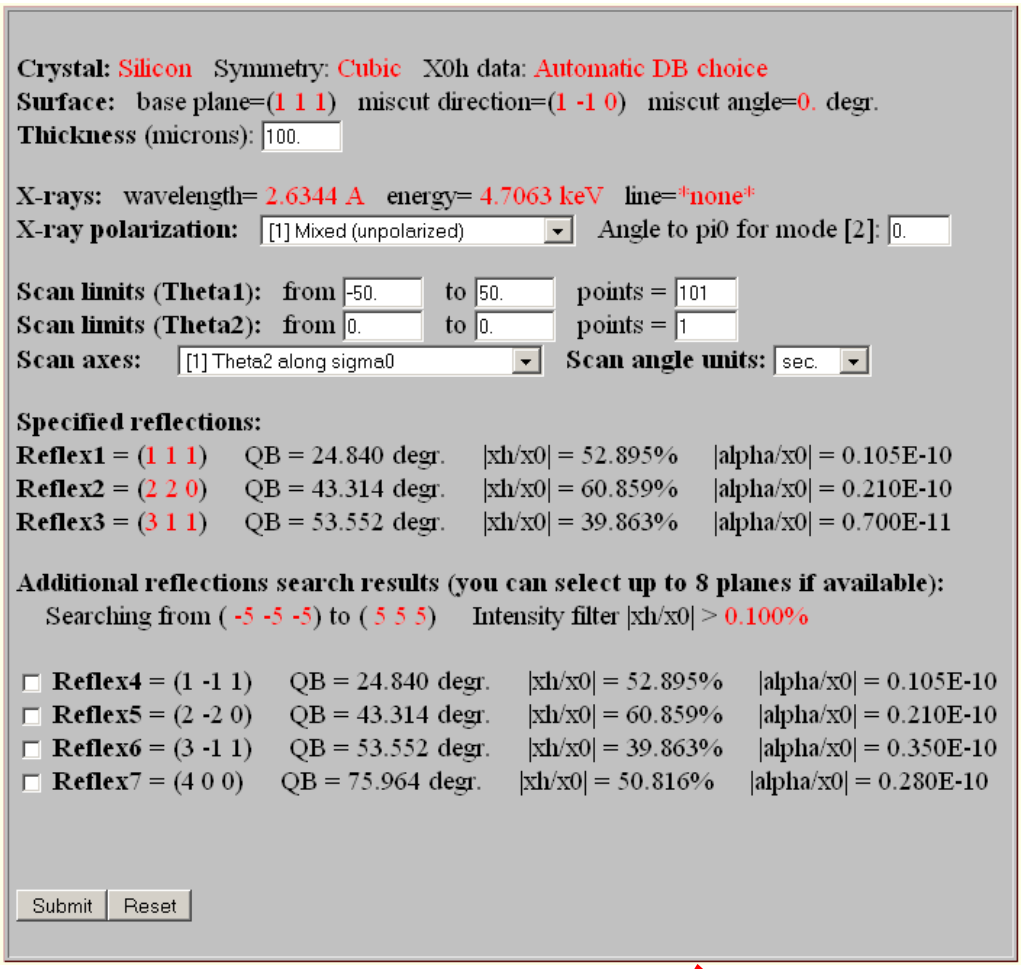
Multiple diffraction program BRL web interface

BRL on the Web
X-ray multiple Bragg/Laue diffraction





Step-1

Step-2

- Step-1 helps finding multiple diffraction configurations and Step-2 defines Bragg scans around arbitrary axes
- **Applications**: X-ray optics (multiple diffraction effects including polarization glitches in X-ray monochromators)

Plans:

- Improve algorithm for thick crystals (provide better numerical stability).

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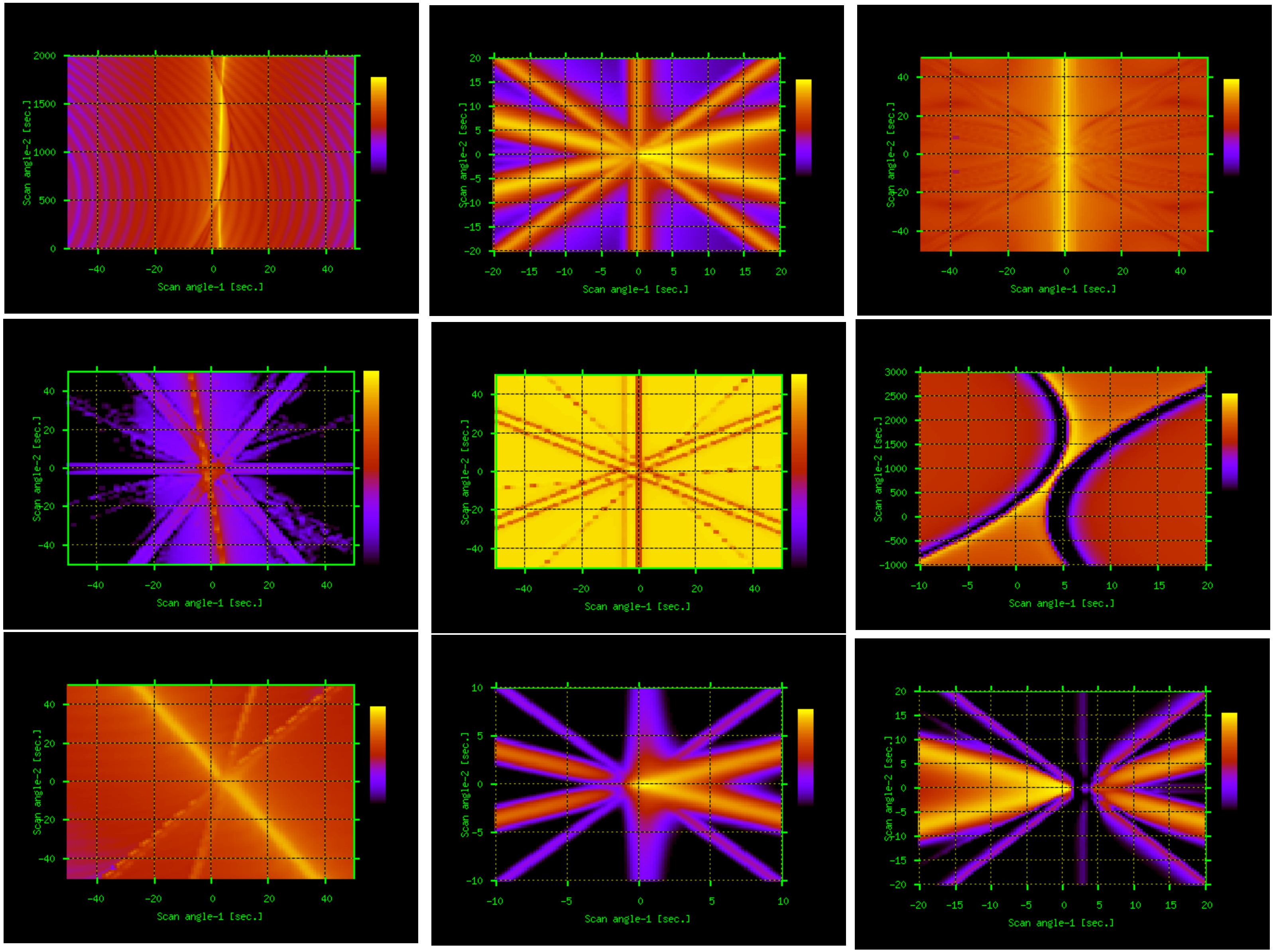
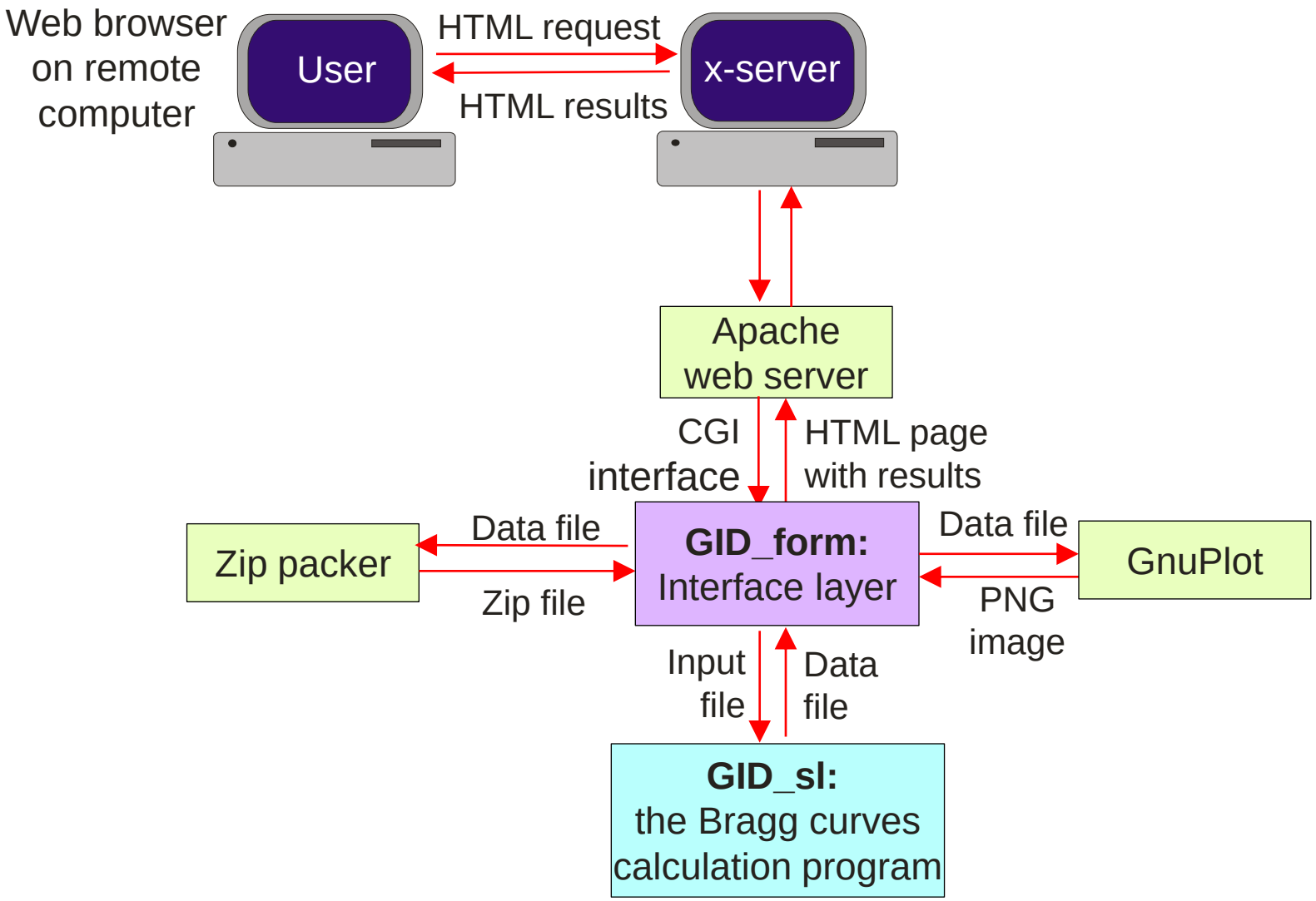
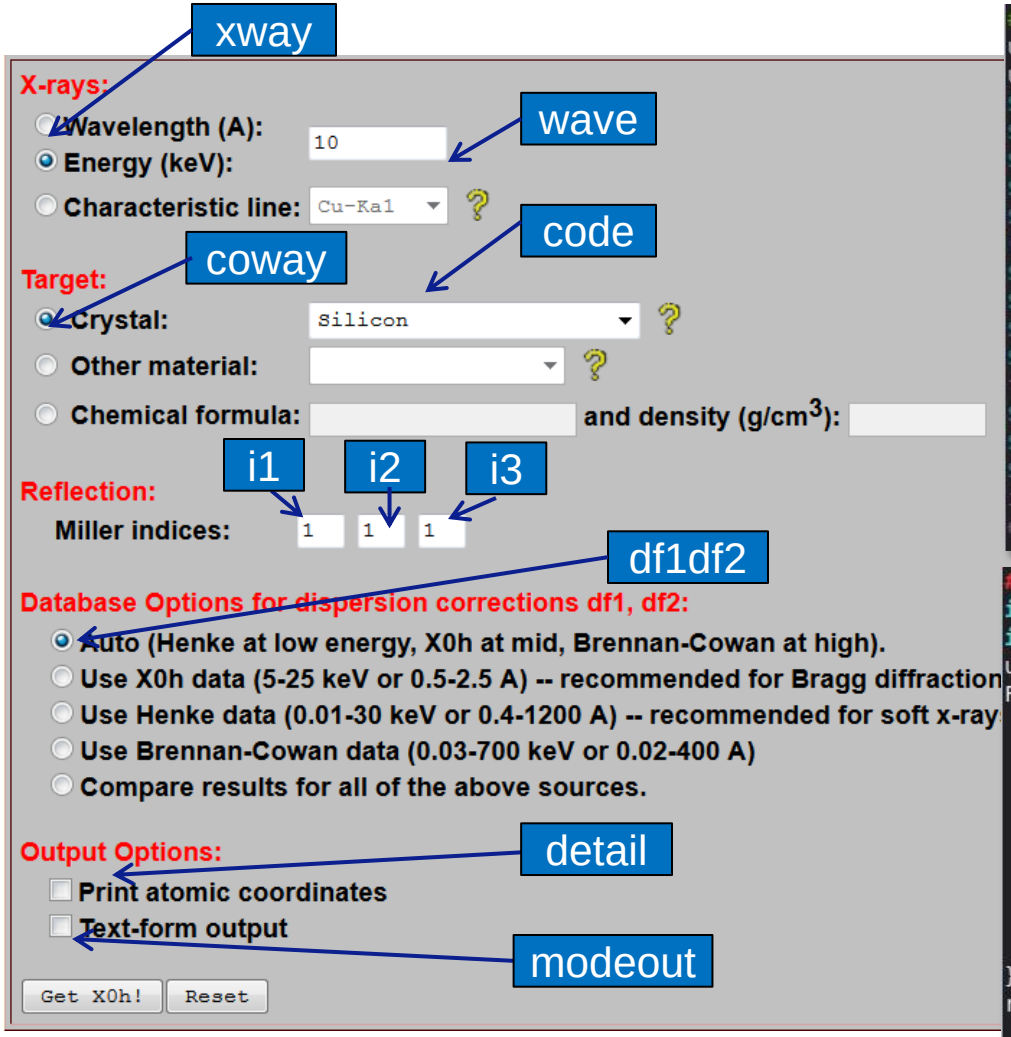
Multiple diffraction program BRL examples



How X-ray Server works



Server access is not limited to web browsers




```perl
#!/usr/bin/perl
use LWP::UserAgent;
use LWP::Protocol::https;
$url = 'https://x-server.gmca.aps.anl.gov/cgi/x0h_form.exe';
$FORM{'xway'} = 2;
$FORM{'wave'} = 10;
$FORM{'coway'} = 0;
$FORM{'code'} = 'Silicon';
($FORM{'i1'},$FORM{'i2'},$FORM{'i3'}) = (1, 1, 1);
$FORM{'df1df2'} = -1;
$FORM{'detail'}  = 0;
$FORM{'modeout'} = 1;
$request = '';
foreach $key (keys %FORM) {$request .= '&'.$key.'='.$FORM{$key};}
$request =~ s/^\&/\?/;
$ua = LWP::UserAgent->new;
$response = $ua->get($url.$request);
if ($response->is_success) {print $response->content;}
else {printf '*** Error: %s'."\n", $response->status_line;}
```

```python
#!/usr/bin/python
import requests
import sys
url = 'https://x-server.gmca.aps.anl.gov/cgi/x0h_form.exe'
FORM = {
    'xway': 2,
    'wave': 10,
    'line': '',
    'coway': 0,
    'code': 'Silicon',
    'i1': 1, 'i2': 1, 'i3': 1,
    'df1df2': -1,
    'detail': 0,
    'modeout': 1
}
response = requests.get(url, params=FORM)

if not response.ok:
    print(f"\n*** Error from the server: {response.status_code}")
else:
   print(response.text)
```

```bash
!#/bin/bash
url=https://x-server.gmca.aps.anl.gov/cgi/x0h_form.exe
curl ${url}?xway=2\&wave=10\&coway=0\&code=Silicon\&i1=1\&i2=1\&i3=1
```

- Python scripts were generated from Perl with the help of AI

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Downloadable examples of X-ray Server access scripts

https://x-server.gmca.aps.anl.gov/automation.html

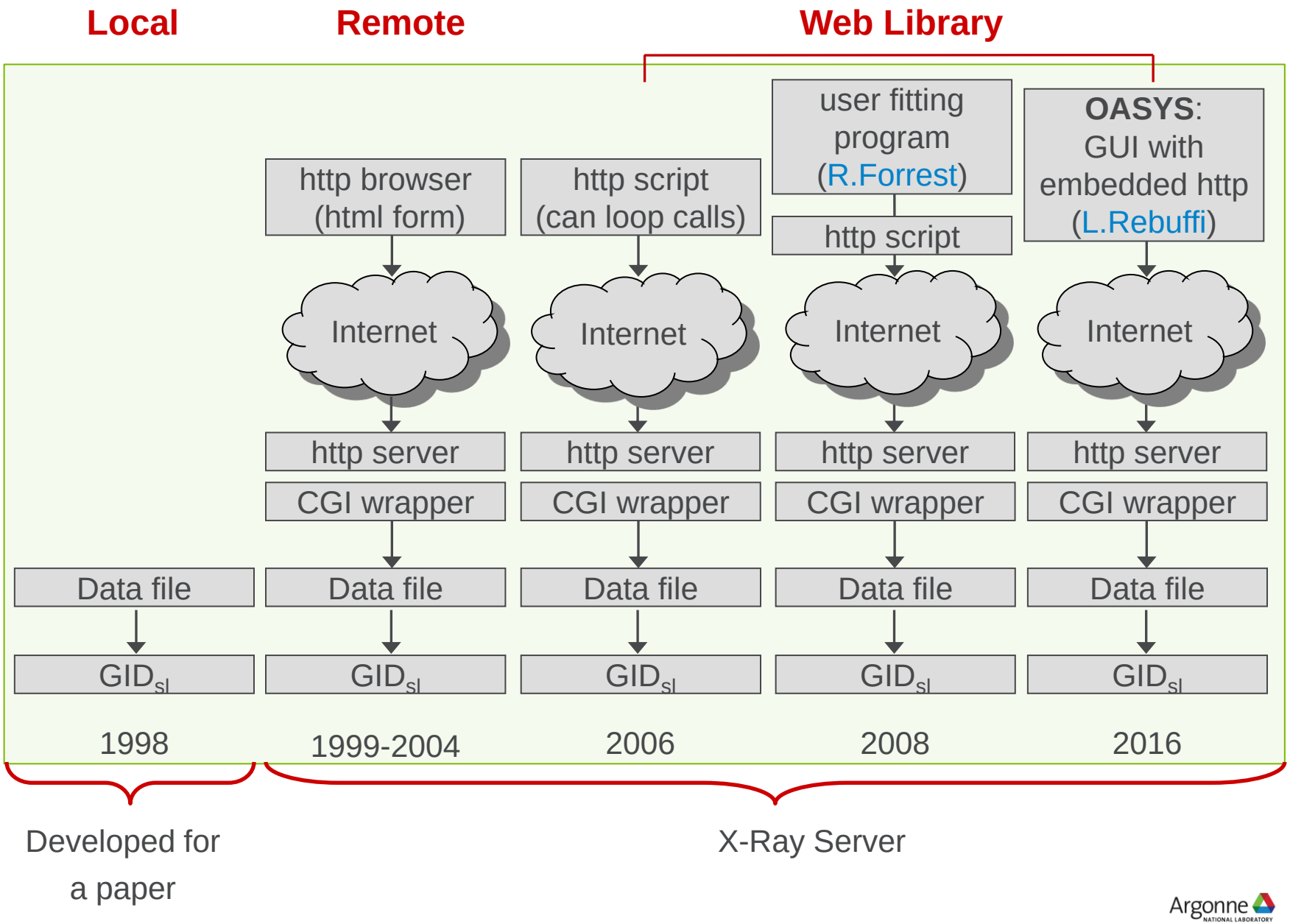
Program	Python script	Perl script
X0h web interface	**getX0h.py**	**getX0h.pl**
GID_sl web interface	**getGID_query_post.py**	**getGID_query_post.pl**
TER_sl web interface	**getTER_query_post.py**	**getTER_query_post.pl**

The scripts can be called from user's software written in any language using the **system** function. If one needs to vary a parameter, it can be passed to the script as a command line argument.

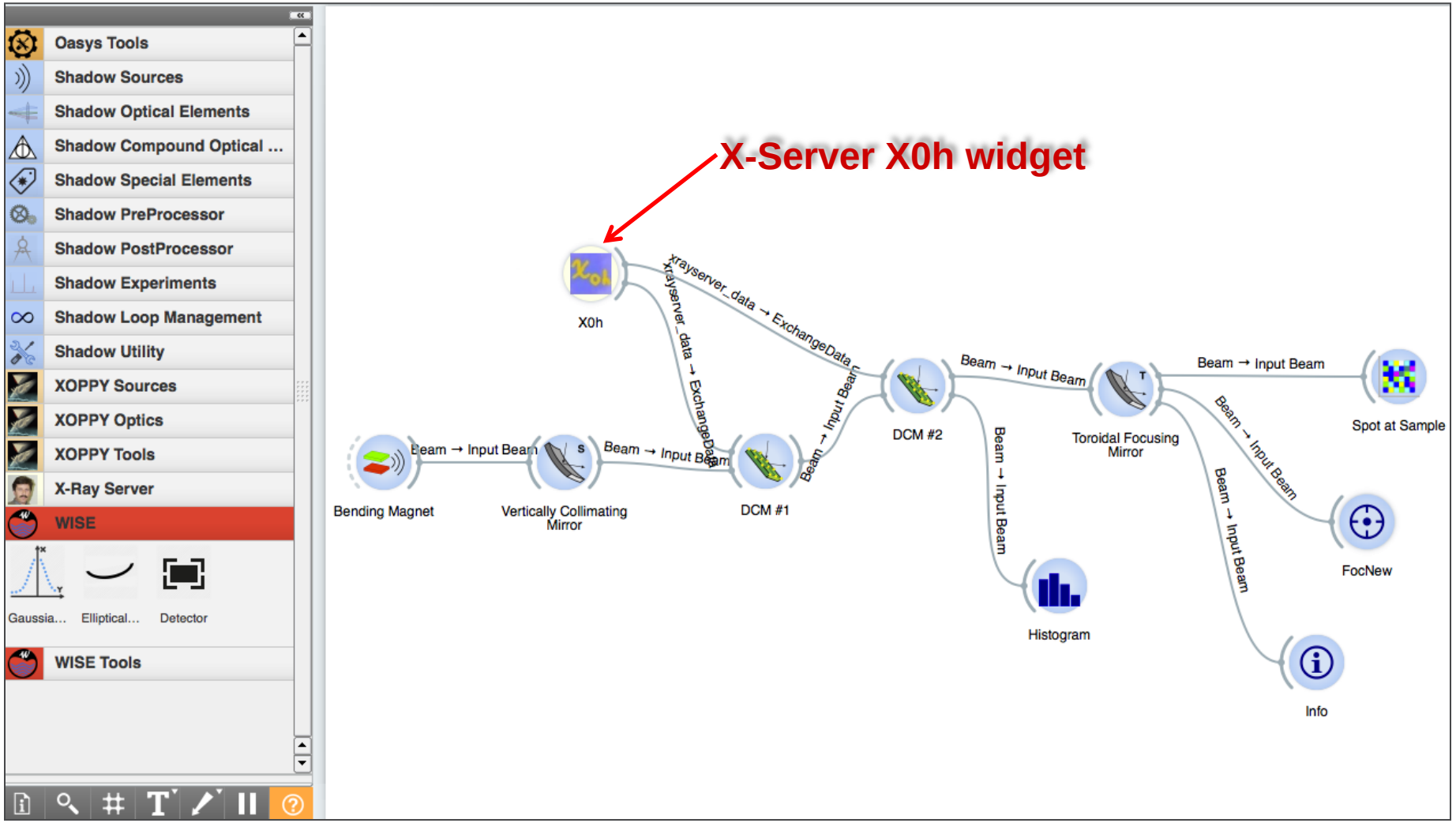
These scripts present a practical example of client software accessing the server programs. They are simple, but they **should be simple** to become useful since they target wide auditory of physicists including those who are unexperienced in web interfaces.

With such scripts X-ray Server can be used as a web-based software library

X-ray Server as a library: evolution



OASYS: new level of interaction with X-ray Server



X-ray Server access is embedded into Oasys and user does not need to do any programming; just add the X-ray Server widgets to your Oasys project.

Courtesy: Dr. Luca Rebuffi

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Some statistics of X-ray Server usage

Frequent users per main programs

Program	Calculations	Total IP addresses	IPs using 100+ times
X0h	3,220,491	22,662	698
GID_sl	1,947,106	10,523	658
TER_sl	426,121	6,328	150

Ten top IP domains most frequently using X-ray server

Nr	ID Domain (number if IPs)	Calculations
1	**desy.de** (1190)	945,608
2	**stanford.edu incl. SLAC/SSRL** (822)	816,867
3	**kit.edu incl. ANKA** (514)	718,713
4	**uh.edu** (97)	348,973
5	**lu.se + lth.se** (340)	290,966
6	**utwente.nl** (263)	20,643
7	**synchrotron-soleil.fr** (7)	19,858
8	**psi.ch** (212)	17,350
9	**esrf.fr (16)**	17,301
10	**anl.gov** (483)	16,488

DESY is #1. Need to add many calls from home and cell ISPs with Geo location in Hamburg

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Conclusions

- We have a well refined resource for the calculations of X-ray dynamical diffraction, specular reflection and diffuse scattering with almost 30 years of online history.
- The main applications are X-ray optics and X-ray material science.
- To get most of this resource, e.g. implement data fitting, one needs to use tools beyond web browser.
- Python and Perl fully functional examples are provided to write such tools on your own, and for some tasks one can use already developed tools like Oasys plugin by Dr. Luca Rebuffi.
- Users are invited to share the tools they developed: these tools can be hosted on the server for the benefit of the whole community – same way as any user-submitted structures are available to everyone using the server.
- Users are welcome to submit new crystals to the server DB and soon they will be able to do it automatically
- Several improvements for the X0h, TER_sl and BRL programs are in plans

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