

QENS at PSI: user's and instrument scientist's point of view

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PSI fit: first impression

```
no file read
```

```
fit>dat 2015/1587, 1600, 1616
```

```
run number(s) without instrument enter  
enter the instrument or project name:  
/afs/psi.ch/project/sinqdata/2015/focu  
lambda= 6.00; Temp= 300.01; Monitc  
Npkt= 1070; owner='Fanni'; Title='2014  
sample='muci_100RH 300K 6AA 1:3'
```

```
/afs/psi.ch/project/sinqdata/2015/focu  
lambda= 6.00; Temp= 150.00; Monitc  
Npkt= 1070; owner='Fanni'; Title='2014  
sample='muci_100RH 150K 6AA 1:3'
```

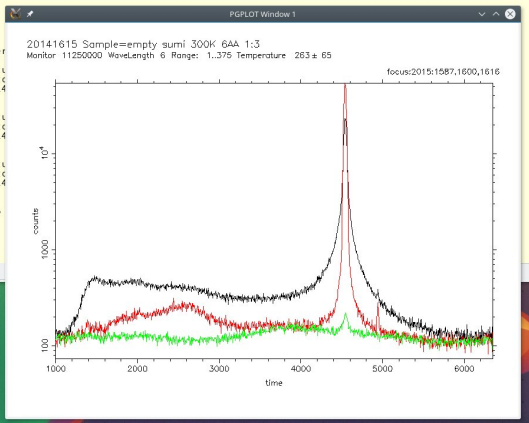
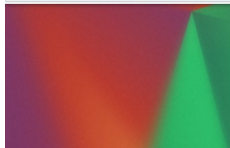
```
/afs/psi.ch/project/sinqdata/2015/focu  
lambda= 6.00; Temp= 300.00; Monitc  
Npkt= 1070; owner='Fanni'; Title='2014  
sample='empty sumi 300K 6AA 1:3'
```

```
Files read: focus:2015:1587,1600,1616
```

```
fit>p
```

```
□
```

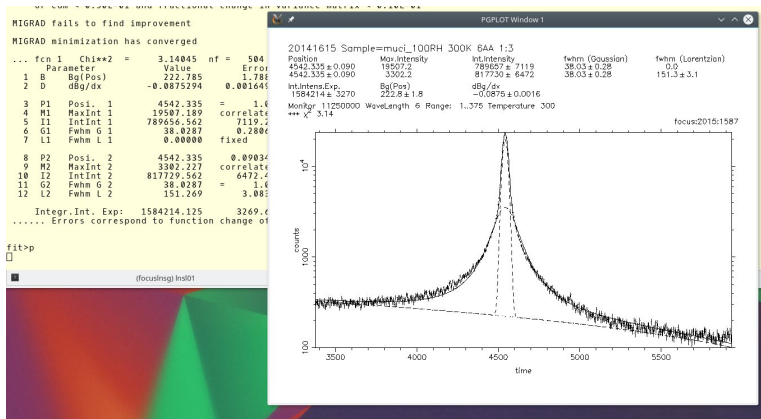
```
(focusnsg) Insl01
```



👉 simple, quick

👉 one more software

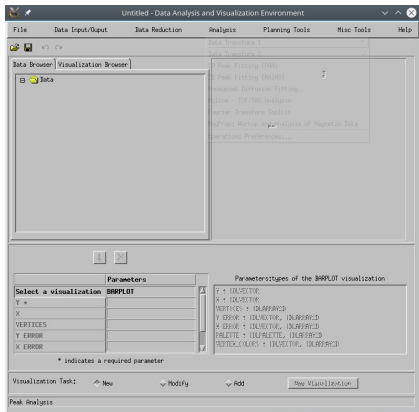
PSI fit: first impression



➤ good combination of terminal and graphical inputs

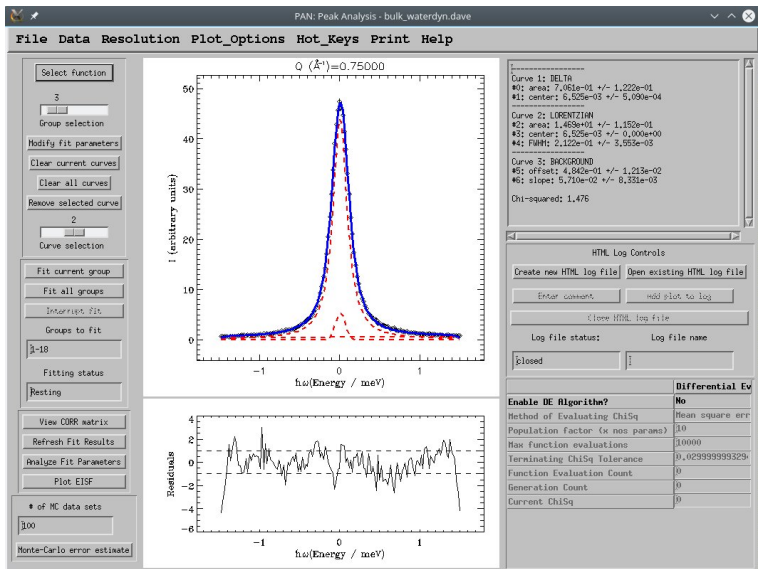
➤ only Voigt + bg

Dave from NIST



- modular structure
- platform independent
- good documentation, tutorial

- heavy weight (modules not selectable)
- widget based, lower level missing
- plotting, limited “matrix” arithmetics
- as grown
- conflicts: discrepancies in ascii format, “raw” and “working” directories
- IDL licence needed for modification
- unconvenient for multi-user or multi-project usage



PAN macro

```
parmnames = ['gammat','gammar','areaw','areat','bg','center']  
gammat = parms[0] & gammar = parms[1] & areaw = parms[2] &  
areat = parms[3] & bg = parms[4] & center = parms[5]
```

...

```
a0 = (sph_bessel(Qgroup * 0.98, 0))2
```

...

```
delta_params = [[areat,center]]
```

```
ymodel = bg + areaw*(a0*yI0 + a1*yI1 + a2*yI2)
```

Values	Fixed	Set Low	Lower Limit	Set High	Upper Limit	Tie
gammat 1.0000000	<input type="checkbox"/> gammat	<input type="checkbox"/> gammat	gammat 0.000000	<input type="checkbox"/> gammat	gammat 0.000000	<input type="checkbox"/> gammat

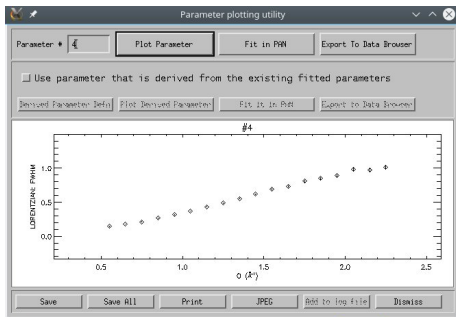
Apply and Dismiss

PAN Parameter Information

LORENTZIAN

Values	Fixed	Set Low	Lower Limit	Set High	Upper Limit	Tie
area 34.570416	<input type="checkbox"/> area	<input type="checkbox"/> area	area 0.00000	<input type="checkbox"/> area	area 0.00000	<input type="checkbox"/> area
center 0.00535628	<input type="checkbox"/> center	<input type="checkbox"/> center	center 0.00000	<input type="checkbox"/> center	center 0.00000	<input type="checkbox"/> center
FWHM 0.21507547	<input type="checkbox"/> FWHM	<input type="checkbox"/> FWHM	FWHM 0.00000	<input type="checkbox"/> FWHM	FWHM 0.00000	<input type="checkbox"/> FWHM

to calculate Lower limits as - 50 % and Upper Limits as + 50 % of current Values



- 👍 userfriendly
- 👍 free user function
- 👍 fit model construction
 - ▶ resolution
 - ▶ parameter handling
- 👎 fit robustness
- 👎 collective fit is missing
- 👎 comparison of different fits

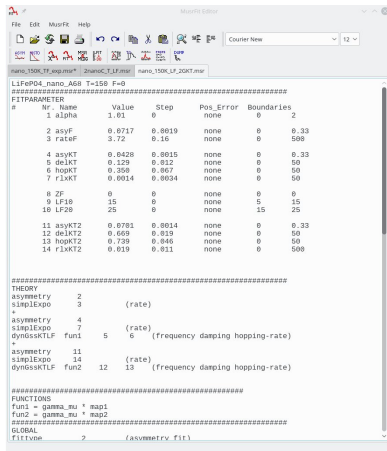
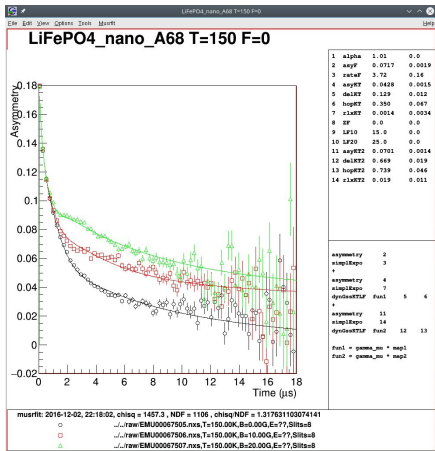
lamp (back in time)

- 👉 workspaces
- 👉 flexible operations
- 👉 easy programming
- 👎 chaos of scripts
- 👎 limited number of workspaces
- 👎 portability

ida

- ▶ command line based
- ▶ number of fit functions
- 👉 common operation on selected workspaces

PSI musrfit



- 🟢 stable results, if converges
- 🟢 global fit

- 🔴 formal constrains
- 🔴 learning curve

small scripts, providing direct access to the raw data

- ▶ Reporting
- ▶ Diagnostics
- ▶ Data treatment, e.g. FWS

#T	num	inel	i	i1	i2	i3	i4	i5	i9	i10	mon	sum mon
297.11	1847	476	1301	54	58	92	109	899	60	29	200000	199951
296.90	1848	439	1355	56	82	106	98	900	76	37	200000	199942

- 🟢 very efficient and felxible
- 🔴 again another software...
- ▶ MSD just an emergency solution

Realization remarks

Users:

- ▶ Info buttons: what is behind the black box?
- ▶ Selectable modules in a common frame, offered at all instruments
- ▶ Small sister/assistant?
- ▶ Common AND definable data formats
- ▶ Easy combination of measurements
- ▶ Self-explaining “click&go” AND terminal programming
- ▶ Trendy design

Instrument scientists (additionally):

- ▶ Flexibility / low level access
- ▶ Personalisation
- ▶ Small sister/assistant?