

Can we learn from **Frida**

for future **f**lexible **r**apid **i**nelastic **d**ata **a**nalysis software?

Joachim Wuttke, MLZ Scientific Computing Group

MLZ is a cooperation between



# Frida



a Swiss Army Knife for  
fast/flexible reliable/rapid inelastic/ingenious data analysis

## History:

- 1990–2001 **Ida** → **Frida1** in Fortran77
- 2001– **Frida2** in C++

# Frida



a Swiss Army Knife for  
fast/flexible reliable/rapid inelastic/ingenious data analysis

## Usage:

- used by a few groups
- taught to users of SPHERES

# Frida



a Swiss Army Knife for  
fast/flexible reliable/rapid inelastic/ingenious data analysis

Status:

- legacy one-man project
- not an official project of MLZ Scientific Computing Group

# Frida



a Swiss Army Knife for

fast/flexible reliable/rapid inelastic/ingenious data analysis

## Has

- open-source licence
- download page, CMake
- version control
- frequent releases
- some tutorials
- some tests

## Hasn't

- GUI
- user manual
- full test coverage

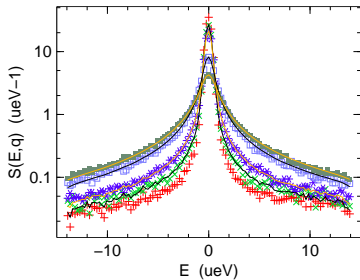
# Frida



a Swiss Army Knife for

fast/flexible reliable/rapid inelastic/ingenious data analysis

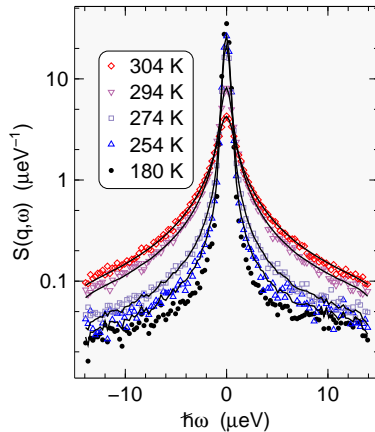
- a collection of algorithms
- operating on data files in RAM («workspaces»)
- controlled by a concise (cryptic) command-line interface
- with dedicated fit models for QENS
- generating human editable PostScript graphics



```
gly5
mfj # gly5 is merger of:
- gly295
glycerol
measured on SPHERES by J.Wuttke
reduced data set for Frida tutorial
fs gly255.y08 # Fri Aug 10 16:16:30 2012
mpaf 3
mr j==8
- gly275
==fs gly275.y08 # Fri Aug 10 16:16:31 2012
- gly295
==fs gly295.y08 # Fri Aug 10 16:16:31 2012
- gly305
==fs gly305.y08 # Fri Aug 10 16:16:31 2012
+ 0 254.107 1.41697
x 1 274.146 1.41697
* 2 293.905 1.41697
□ 3 304.177 1.41697
fit_gly5
```

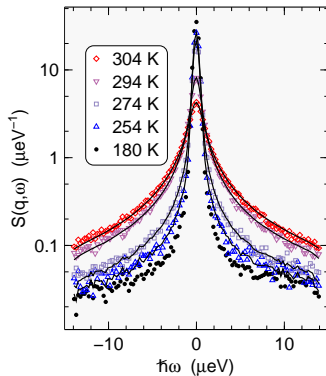
```
cc p0*pconvp(kwvp(t.p1,p2)) # z from gly5
p0*pconvp(kwvp(t.p1,p2))
data file: 14, conv file: 13, weighing: with reciprocal variance (data and curve)
| z0 z1 p0 p1 p2 oc chi^2 1-R^2
- 0 254.107 1.41697 24.1952 292.671 0.414796 1 1.80418 0.134212
- 1 274.146 1.41697 23.3787 22.3248 0.484547 1 3.21818 0.352675
- 2 293.905 1.41697 21.9556 1.25831 0.551861 1 1.21577 0.599272
- 3 304.177 1.41697 20.9664 0.521076 0.586763 1 1.34236 1.75922
```

plot -> /home/wu/pub/V/17/1704-Frida-gly\_join.ps

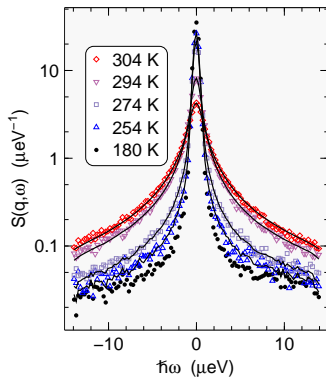


8 minutes manual editing

```
.8 3.9 5.1 8.8 .2 oval
  { white fill } G 1 [] lset st
.9 8.4 24 1.8 NewList
5 {(304 K)} PtTxLine
4 {(294 K)} PtTxLine
3 {(274 K)} PtTxLine
2 {(254 K)} PtTxLine
1 {(180 K)} PtTxLine
```







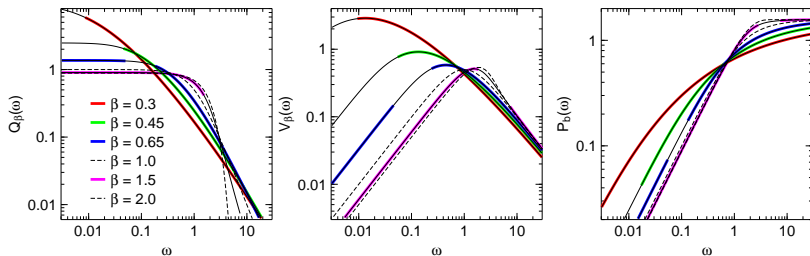
```

1 [ 254.107 1.41697 ] zValues
1 pstyle % (E (ueV) -> S(E,q) (ueV-1))
0.36000 1.58792 0.21947 ti % -13.92 wx 0.04215903 wy
0.44000 1.46066 0.23179 t % -13.68 wx 0.03785536 wy
0.52000 1.81438 0.19977 t % -13.44 wx 0.051063 wy
[...]
```

Article

# Laplace–Fourier Transform of the Stretched Exponential Function: Analytic Error Bounds, Double Exponential Transform, and Open-Source Implementation “libkww”

Joachim Wuttke

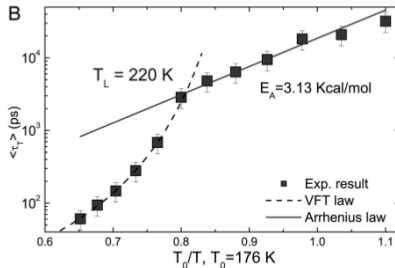
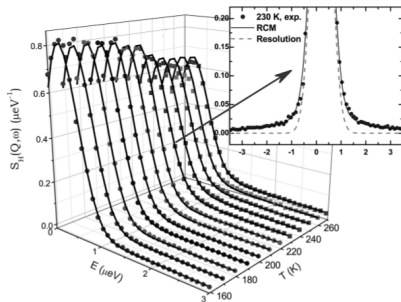


# Observation of fragile-to-strong dynamic crossover in protein hydration water

S.-H. Chen<sup>\*†</sup>, L. Liu<sup>\*</sup>, E. Fratini<sup>‡</sup>, P. Baglioni<sup>‡</sup>, A. Faraone<sup>§¶</sup>, and E. Mamontov<sup>§¶¶</sup>

<sup>\*</sup>Department of Nuclear Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139; <sup>†</sup>Department of Chemistry and Consorzio Interuniversitario per lo Sviluppo dei Sistemi a Grande Interfase (CSGI), University of Florence, via della Lastruccia 3, 50019 Florence, Italy; <sup>‡</sup>NIST Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD 20899-8562; and <sup>§</sup>Department of Materials Science and Engineering, University of Maryland, College Park, MD 20742-2115

Communicated by H. Eugene Stanley, Boston University, Boston, MA, March 28, 2006 (received for review March 11, 2006)



## Dynamical Transition of Protein-Hydration Water

W. Doster,\* S. Busch, and A. M. Gaspar

*Physik Department E 13 and ZWE FRM II, Technische Universität München, 85747 Garching, Germany*

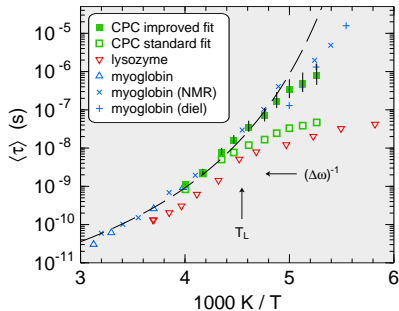
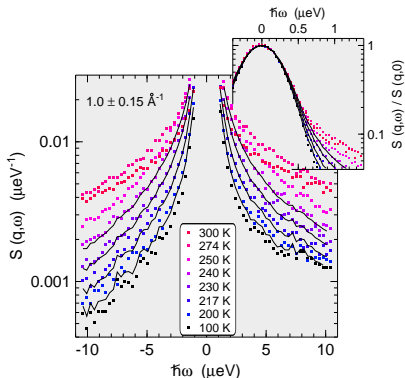
M.-S. Appavou and J. Wuttke

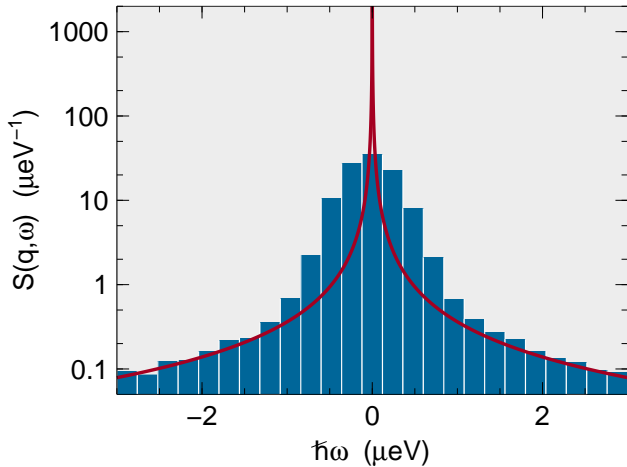
*Forschungszentrum Jülich, JCNS at FRM II, Lichtenbergstrasse 1, 85747 Garching, Germany*

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(Received 22 July 2009; published 2 March 2010)





$$(R \otimes T)(\omega) = \sum_{\omega'} R(\omega - \omega') T(\omega')$$

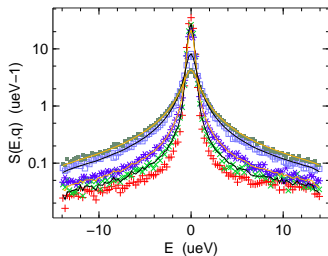
must be replaced by

$$(R \otimes T)(\omega) = \sum_{\omega'} R(\omega - \omega') [P(\omega' + \Delta\omega/2) - P(\omega' - \Delta\omega/2)]$$

```

fl g*
msr! 8
mpaf! 3
1:4 mfj
1:4 fdel
1 cc p0*pconv(kwwp(t,p1,p2))
cv 0
2 op2 .6
cx 2
cf
cu 2
cf
g2
0 p
1:2 a :
gp graphic_file_name

```

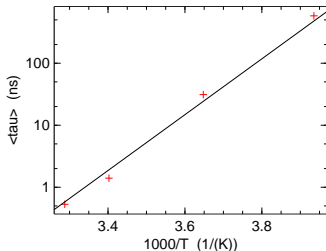


gly180  
glycerol  
measured on SPHERES by J.Wuttke  
reduced data set for Frida tutorial  
ls gly180.y08 # Fri Aug 10 16:16:30 2012  
mpaf 3  
+ - 1.41697  
gly255  
...

```

2 oi .6582*p1/p2*gamma(1/p2)
ecy <tau>(ns)
ox! 1000/x
cc p0*exp(p1*t)
cwl
cf
ga
3,4 p
gp graphic_file_name

```



```

fit_gly5
cc p0^pconv(kwvp(lp1_p2)) # z from gly5
oi .6582*p1/p2*gamma(1/p2)
ecy <tau>(ns) # old: 0.658200*p1/p2*gamma(1/p2)
ox 1000/x
+ 0
fit_fit_gly5
cc p0*exp(p1*t) # z from fit_gly5
p0*exp(p1*t)
data file: 5, weighing: logarithmic
j p0 p1 cc chi^2 1--R^2
- 0 9.1608e-16 10.367 5 0.203248 8.32178e-07
plot -> /home/ysu/pub/V/17/1704-Frida/gly-tau.ps

```

y is shorthand for y[, ] is shorthand for y[k, j, i]

Command `oy f(y)` is executed as

```
for k in file_selection:
    for j in [0,nj) spectra in file
        for i in [0,ni) points in spectrum
            y_out[k_out, j, i] := f(y[k, j, i])
```

This allows for

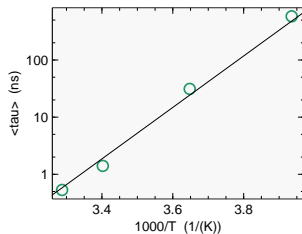
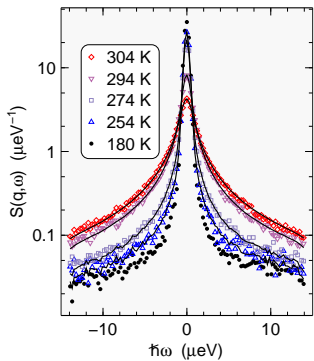
`oy y/y[0]` *normalize to file 0*

`oy y/y[,0]` *normalize to spec 0 of current file*

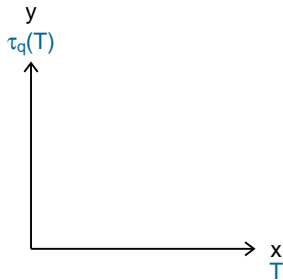
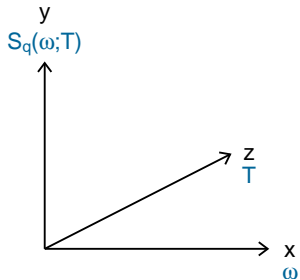
`oy y/y[, ,0]` *normalize to point 0 of current spec*

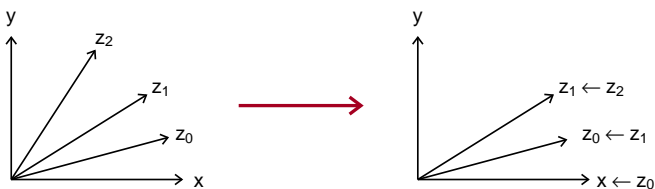
`oy y/y[k-4,0, j]` *normalize spec j to point j of spec 0 of file k-4*





extract fit parameter  
 reduce dimension  $\rightarrow$





### Dimension-reducing operations:

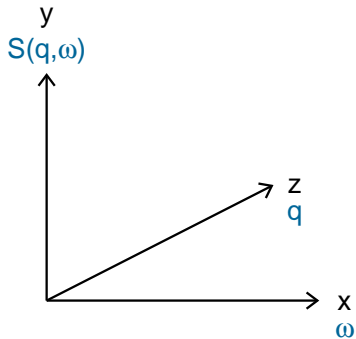
<code>p0</code>	fit parameter 0
<code>ni</code>	number of points in spectrum
<code>sum(y)</code>	$\sum y[, i]$
<code>avge(y)</code>	$\sum y[, i] / ni$
<code>integral(x, y)</code>	$\int dx y(x)$ per midpoint rule
<code>valmax(y)</code>	$\max_i y[, i]$
<code>idxmin(y)</code>	index $i$ for which $y[, i]$ is minimal
<code>cog(x, y)</code>	center of gravity in $x$ weighed with $y$
<code>width(x, y)</code>	standard variation in $x$ weighed with $y$
<code>corr(x, y)</code>	correlation coefficient of $x$ and $y$
<code>firstwith(expr)</code>	first $i$ for which <code>expr</code> is true

## Other functionality:

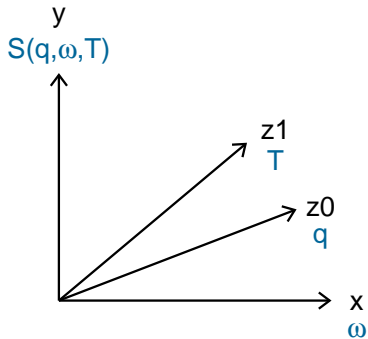
- command line as pocket calculator
- function plotter handling singularities and frame crossings
- function integration
- 2D color plots
- import/export from/to various tabular formats

## Code base:

- < 18k lines C++
- not counting libkww, libcerf
- expressions handled by flex/yacc
- weak encapsulation »we are all consenting adults«
- 1.5k lines PostScript macros



manageable



too complex

most users  
just want to  
press GUI buttons

some users  
want full  
control & understanding



serve them



empower them

most experiments  
can be analyzed  
in routine ways

some experiments  
require closer  
investigation



prevent misuse

*primum non nocere*



automatize further

