



**COherent NUclear Scattering from Single crystals**

**Software for the evaluation of  
Synchrotron Mössbauer Spectra**

Wolfgang Sturhahn

[wolfgang@nrixs.net](mailto:wolfgang@nrixs.net)

# About CONUSS:

- developed 1983-1986 by E. Gerdau and W. Sturhahn at the University of Hamburg
  - ☆ coherent elastic nuclear and electronic Bragg scattering
  - ☆ explain first NRS experiments (Gerdau et al. PRL 54, 1985)
  - ☆ FORTRAN code implemented on IBM 360 mainframe (MVS-VM)
  
- improved 1986-today by W. Sturhahn and supported by the University of Hamburg (1986-1993), ESRF (1992), APS (1992-2010), MPI-Halle (2012-2013)
  - ☆ forward scattering (SMS a.k.a. NFS) added in 1991
  - ☆ ported to Sun UNIX in 1992
  - ☆ extended data handling capability (fitting) added in 1996
  - ☆ ported to Linux in 2004, to OS X in 2011
  - ☆ grazing incidence scattering (GINS) added in 2014

*publications related to CONUSS:*

*W. Sturhahn and E. Gerdau, Phys. Rev. B 49 (1994)*

*W. Sturhahn, Hyperfine Interact 125 (2000)*

## More on CONUSS:

- has been used for data evaluation in numerous publications
- distributed under GPL, source code public, evaluations traceable
- can be obtained at <http://www.nrixs.com> – no charge
- a major upgrade, CONUSS-2.0.0, was released in 2010
  - ☆ simple installation procedure for Unix and Mac OS X
  - ☆ all previous capabilities of CONUSS
  - ☆ enhanced fit capabilities
  - ☆ run-time graphics
  - ☆ new Monte Carlo approach to find start-values, explore the parameter space, and smart parameter optimization
- CONUSS-2.1.0 will be released in 2014
  - ☆ support of grazing incidence geometry
  - ☆ input parameter simplifications
- possible future development
  - ☆ Graphical input file editor

## CONUSS now supports:

- all Mössbauer isotopes
- forward scattering, grazing incidence, and Bragg/Laue reflections
- no limitations by sample structure
- combined hyperfine interactions
- distributions of hyperfine fields
- textures
- relaxation effects
- full polarization and directional dependences
- thickness effects
- time spectra (SMS) and energy spectra (trad. Mössbauer spectr.)
- sample combinations
- time, energy, and angle averaging
- sample thickness distributions
- comparison to experimental data including fitting
- flexible assignment and grouping of fit parameters

# KMCO app screen shot:

The screenshot displays the KMCO application interface on a Mac OS X desktop. The main window shows a plot of counts versus time (ns) for sampling 1721, with a  $\chi^2 = 3.683$ . The plot shows a decaying signal with several peaks. The y-axis is logarithmic, ranging from  $10^2$  to  $10^4$ . The x-axis is linear, ranging from 0 to 140 ns.

The interface includes a terminal window on the left showing the KMCO command-line interface, a file browser on the right showing the contents of the /Users/wsturhah/CONUSS-2.0.1/example... directory, and two Emacs windows at the bottom showing the fit parameters and input files for the 'in\_kmco' module.

**Terminal Window (Terminal - xmgrace - 115x54):**

```
[NFS2]54: conuss mco
++ CONUSS-2.0.1 Copyright (C) 2011 Wolfgang Sturhahn
++ This program comes with ABSOLUTELY NO WARRANTY.
++ This is free software.
++ You may redistribute it under certain conditions.
++ For details see <http://www.gnu.org/licenses/>.

-- CONUSS module KMCO data section size: 48.10 Mb
-- execution starting..

Estimated success probabilities vs. level:
Individual sampling: 3.19E-13 3.16E-11 3.14E-09 3.11E-07 3.09E-05 3.07E-03 3.04E-01 1.00E+00 1.00E+00 1.00E+00
All samplings:      6.37E-11 6.33E-09 6.28E-07 6.23E-05 6.16E-03 4.59E-01 1.00E+00 1.00E+00 1.00E+00 1.00E+00
Number of samplings: 2001

Best samplings:
22.32 2.50E-01 2.48E+00 2.50E-01 1.53E+00 3.00E-01 5.00E-01 6.00E-01 -7.00E-01 4.50E-01 3.75E+04
16.94 2.63E-01 2.38E+00 1.49E-01 1.77E+00 2.82E-01 4.32E-01 3.01E-01 -6.27E-01 6.37E-01 3.76E+04
10.46 3.07E-01 2.44E+00 2.82E-01 1.97E+00 3.09E-01 7.91E-01 3.50E-01 -5.89E-01 4.94E-01 2.02E+04

Entering nesting level 2; using 5 search area(s)
Entering nesting level 3; using 1 search area(s)
8.97 3.53E-01 2.44E+00 2.13E-01 1.95E+00 2.72E-01 7.96E-01 3.48E-01 -6.07E-01 5.05E-01 1.96E+04
7.21 3.50E-01 2.51E+00 2.51E-01 1.82E+00 3.68E-01 7.09E-01 3.69E-01 -5.52E-01 4.58E-01 2.41E+04
6.34 3.78E-01 2.51E+00 2.28E-01 1.82E+00 3.13E-01 6.87E-01 3.54E-01 -5.56E-01 5.34E-01 2.43E+04
5.48 3.31E-01 2.49E+00 2.26E-01 1.91E+00 3.73E-01 7.55E-01 3.54E-01 -5.36E-01 5.54E-01 2.54E+04

Entering nesting level 4; using 3 search area(s)
Entering nesting level 5; using 10 search area(s)
Entering nesting level 6; using 11 search area(s)
5.20 4.12E-01 2.43E+00 2.42E-01 1.67E+00 3.18E-01 7.81E-01 4.66E-01 -5.94E-01 4.90E-01 2.16E+04
4.82 3.61E-01 2.52E+00 1.88E-01 1.88E+00 2.69E-01 7.98E-01 3.74E-01 -5.46E-01 5.22E-01 2.36E+04

Entering nesting level 7; using 8 search area(s)
Entering nesting level 8; using 7 search area(s)
4.16 3.33E-01 2.52E+00 1.72E-01 1.92E+00 2.55E-01 7.56E-01 3.57E-01 -5.54E-01 4.88E-01 2.44E+04
3.88 3.57E-01 2.50E+00 2.10E-01 1.87E+00 2.74E-01 7.87E-01 3.42E-01 -5.54E-01 5.55E-01 2.33E+04

Entering nesting level 9; using 2 search area(s)
3.78 3.56E-01 2.53E+00 2.09E-01 1.87E+00 2.54E-01 7.53E-01 3.58E-01 -5.53E-01 4.87E-01 2.33E+04
3.68 3.54E-01 2.52E+00 2.07E-01 1.88E+00 2.53E-01 7.58E-01 3.55E-01 -5.53E-01 4.86E-01 2.32E+04

Entering nesting level 10; using 34 search area(s)

-- CPU time : user 348.21 s system 0.20 s
-- CONUSS module KMCO finished

[NFS2]55: 
```

**File Browser (1 of 23 selected, 434.13 GB available):**

Name	Size	Kind
fepv_in	12 KB	Document
fepv_in.mco	8 KB	Document
in_kfit	4 KB	Document
in_kmco	4 KB	Document
in_kmiox	4 KB	Document
in_kmiox.mco	4 KB	Document
in_kref	8 KB	Document
in_kref.mco	8 KB	Document
mcochi2.hst	8 KB	Document
mcoparm.hst	8 KB	Document
out_kmco	229 KB	Document
parmi2v3.D	90 KB	Document
parmi2v3.D	115 KB	Document
Perovskite_30GPa.dat10	12 KB	Document
parm01.dat	45 KB	XEmacs Wr...Docume
parm02.dat	45 KB	XEmacs Wr...Docume
parm03.dat	45 KB	XEmacs Wr...Docume
parm04.dat	45 KB	XEmacs Wr...Docume
parm05.dat	45 KB	XEmacs Wr...Docume
parm06.dat	45 KB	XEmacs Wr...Docume
parm07.dat	45 KB	XEmacs Wr...Docume
parm08.dat	45 KB	XEmacs Wr...Docume
parm09.dat	45 KB	XEmacs Wr...Docume

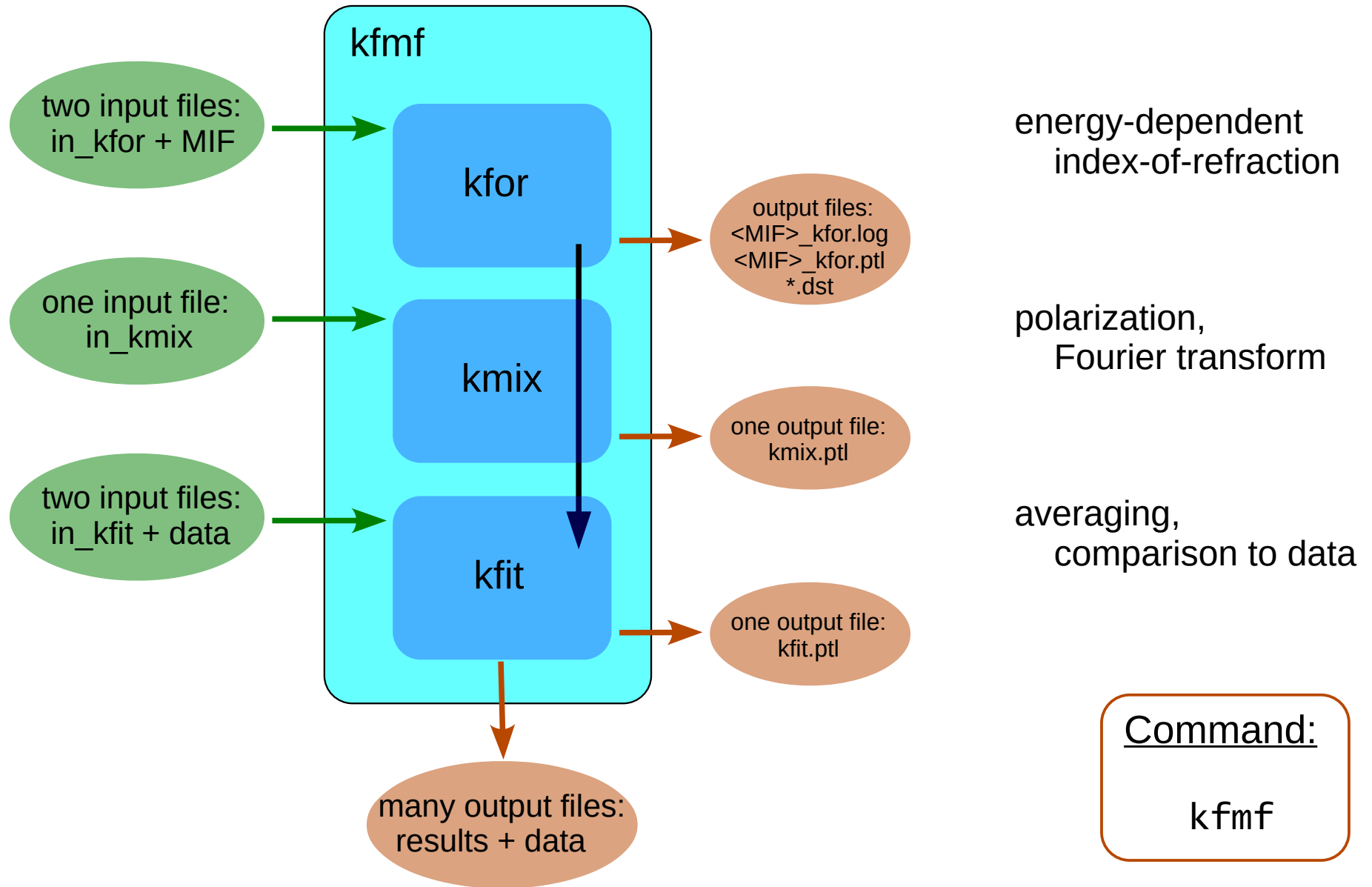
**Emacs: fepv\_in**

```
* fit parameters
* =====
*
* the first number gives the center of parameter search box|
* the second number gives the size of the parameter search box
*
* % @ &wght21 := 0.25 0.2
* % @ &quad21 := 2.48 0.5
* @ &iso21 := 0
* @ &dist21 := 0
*
* % @ &wght22 := 0.25 0.2
* % @ &quad22 := 1.53 0.5
* @ &iso22 := 0
* @ &dist22 := 0.3 0.2
*
* % @ &wght3 := 0.5 0.3
* % @ &quad3 := 0.6 0.3
* % @ &iso3 := -0.7 0.3
* % @ &dist3 := 0.45 0.2
*
* -----1-----2-----3-----4-----5-----6-----7-->
*
* * MB ismtime and MB transiting
IS08----XEmacs: fepv_in (Fundamental PerDel)----L15--C61--4%-----
(No changes need to be saved)
```

**Emacs: in\_kmco**

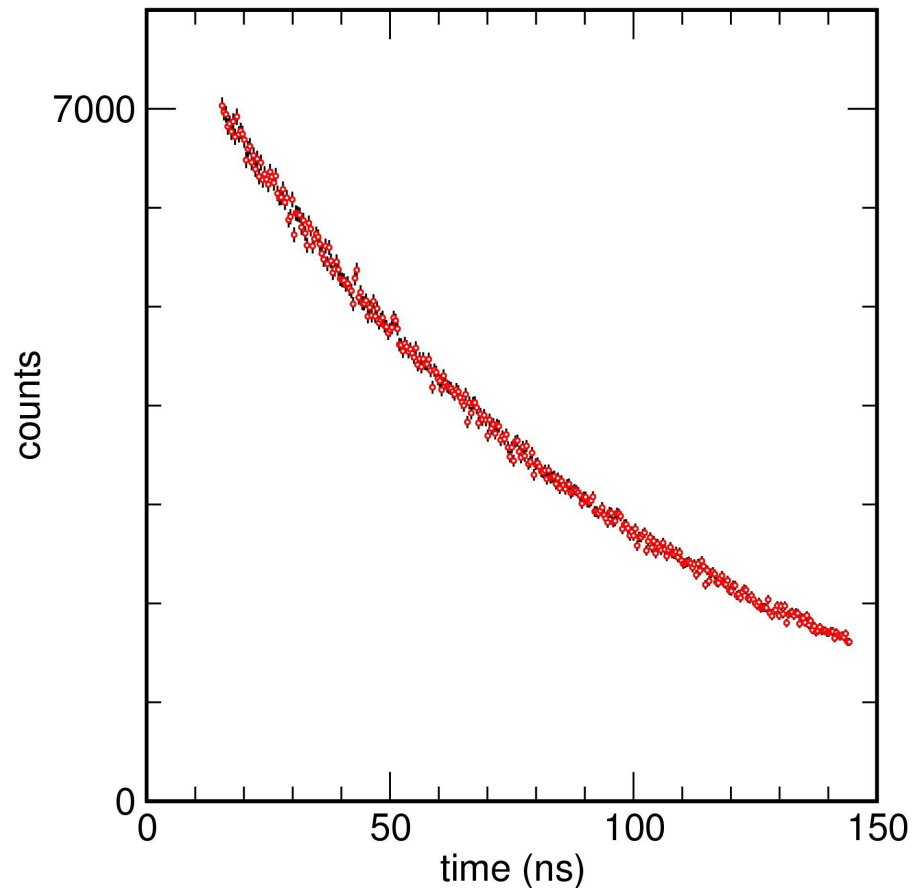
```
* input and output files
* =====
*
* (1) input file for module KREF :: in_kref
* (2) input file for module KMIX :: in_kmiox
* (3) input file for module KFIT :: in_kfit
*
* * sampling|
* =====
*
* (4) number of levels :: 10
* (5) random samples per level :: 200
*
* (6) search box level-reduction factor :: 0,6
* (7) factor for acceptable chi^2 minima :: 3
*
* =====
IS08----XEmacs: in_kmco (Fundamental PerDel)----L37--C10--57%-----
```

# Module configuration, theory and simple fit:



# SMS example 1.1:

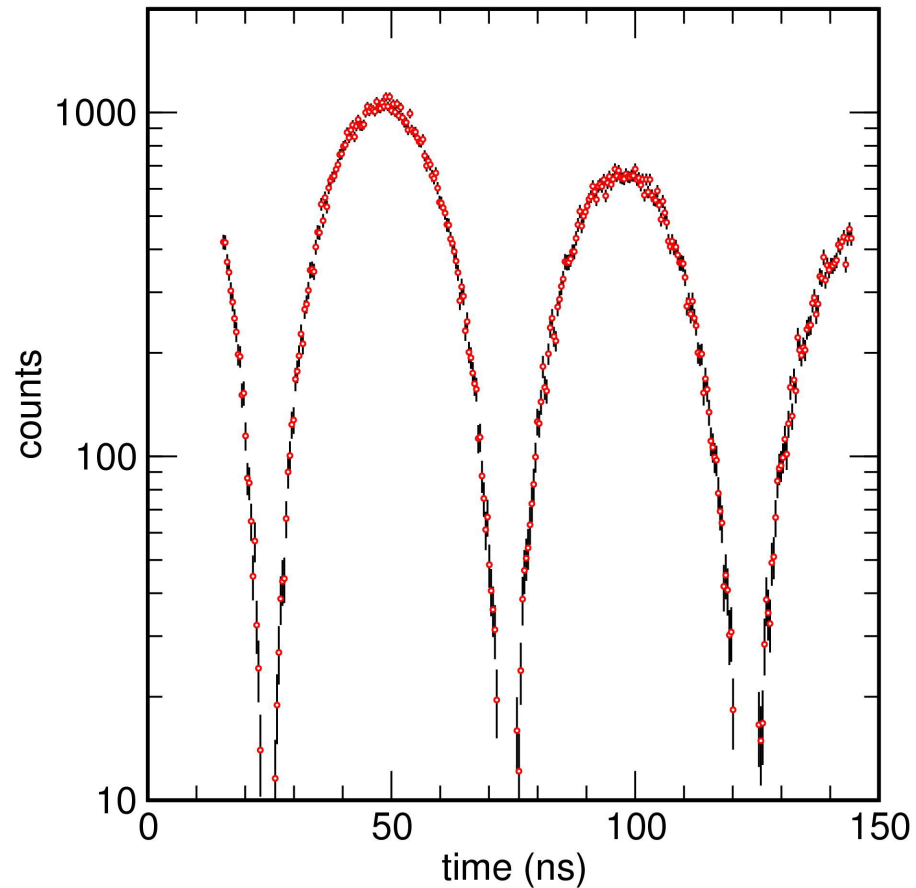
➤ simulate the following SMS spectrum



- ☆ construct the input files  
in\_kfor, in\_kmix, in\_kfit, ex1-1.mif
- ☆ observe the effect of isomer shift,  
thickness, quadrupole splitting
- ☆ Tips: watch correlations

## SMS example 2.1:

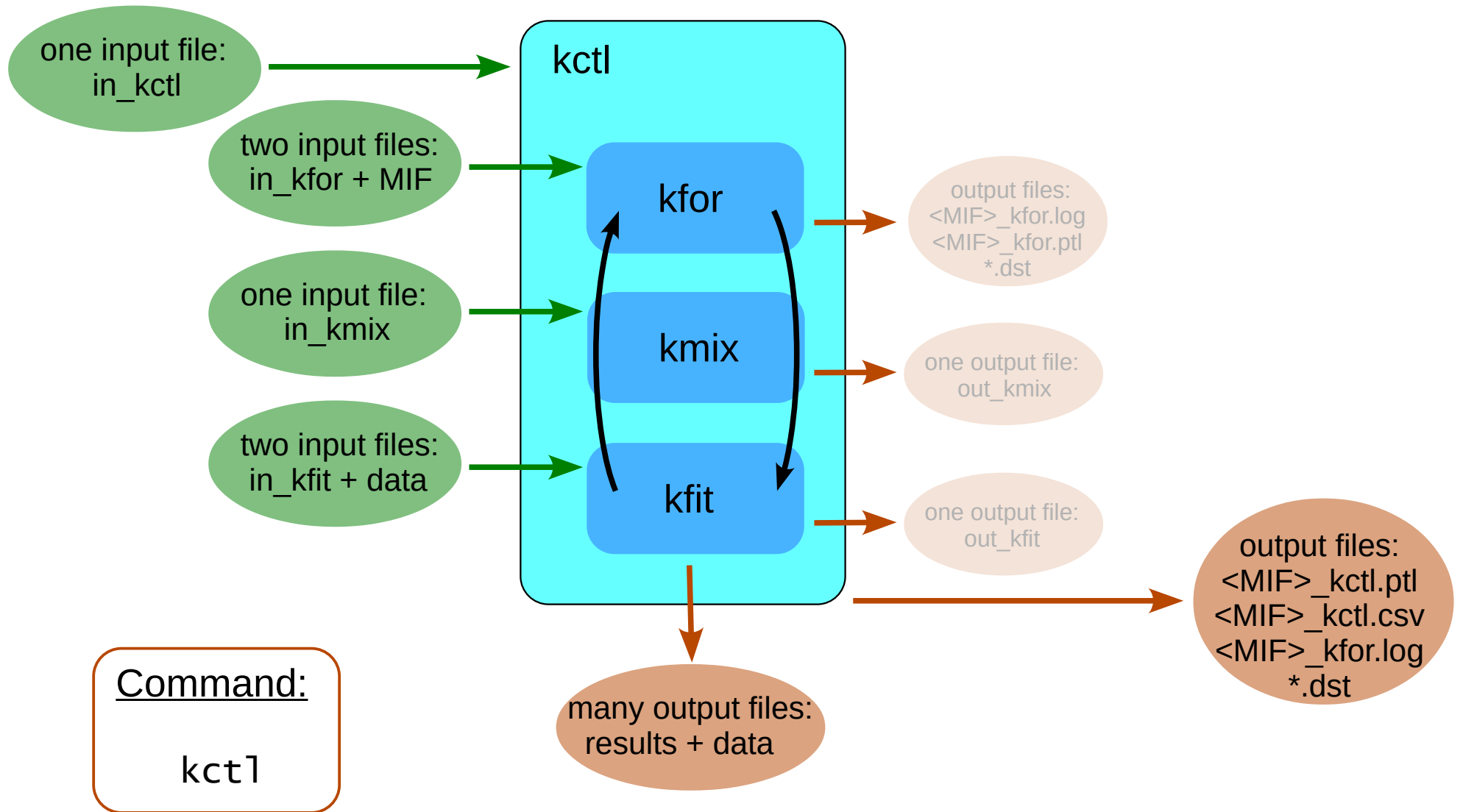
➤ simulate the following SMS spectrum



- ☆ construct the input files  
in\_kfor, in\_kmix, in\_kfit, ex2-1.mif
- ☆ observe the effect of thickness,  
quadrupole splitting
- ☆ Tips: watch correlations



# Module configuration, general fitting:



# Fitting of SMS spectra:

## ➤ strategy

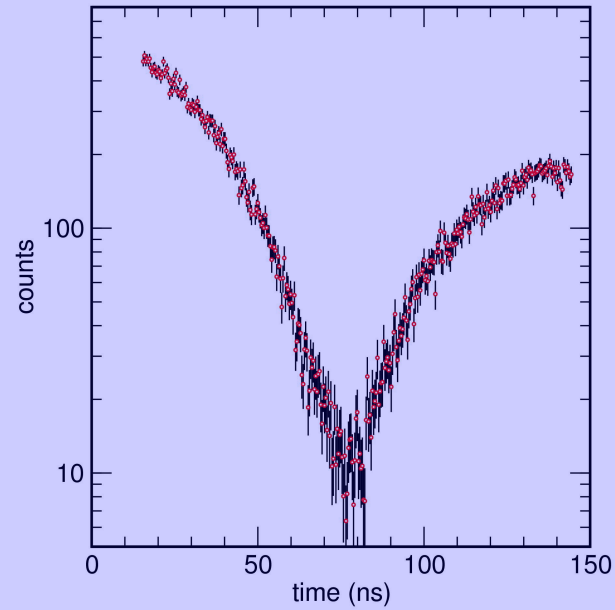
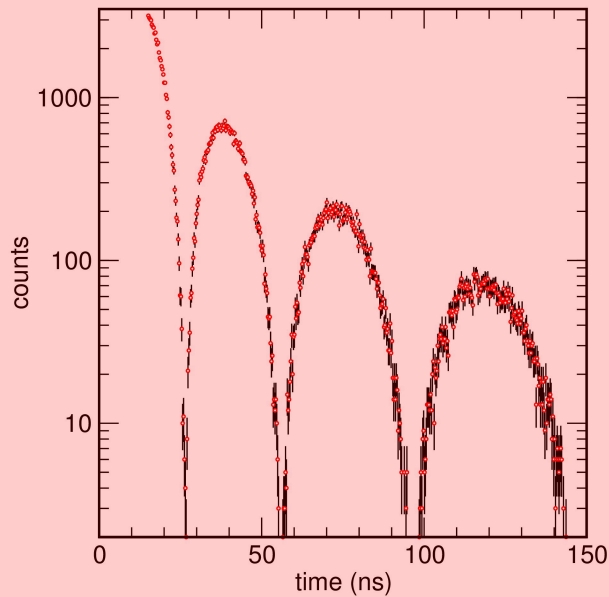
- ☆ identify relevant parameters
- ☆ find start values using command `kfmf`
- ☆ optimize parameter values using `kctl`

## ➤ examples 1.2-4, 2.1-3, and 3.1-3

- ☆ construct the input files `in_kfor`, `in_kmix`, `in_kfit`, `ex.mif`, `in_kctl`
- ☆ focus on isomer shift, thickness, quadrupole splitting

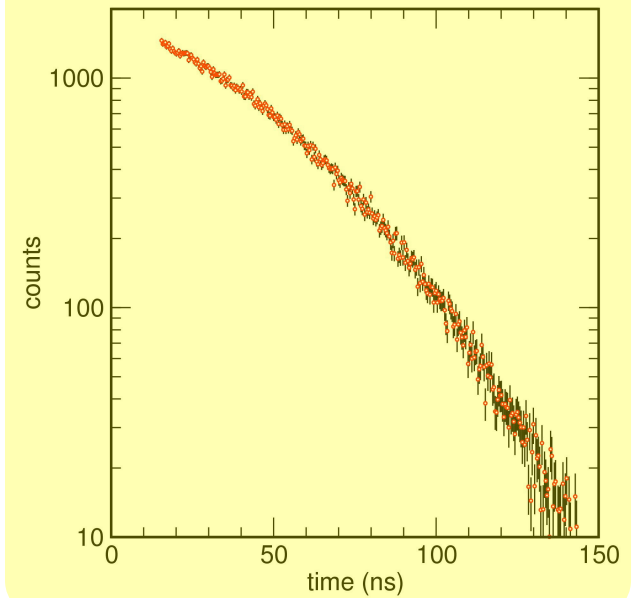
# SMS examples:

- example 1.2  
focus on thickness



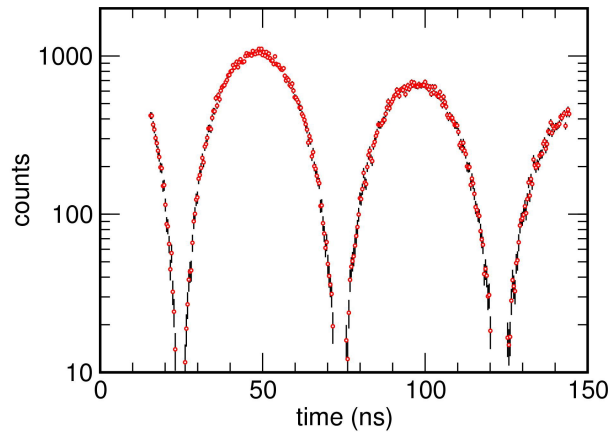
- example 1.3  
two sites; isomer shift;  
thickness  $0.1\mu\text{m}$

- example 1.4  
IS distribution;  
thickness  $0.1\mu\text{m}$

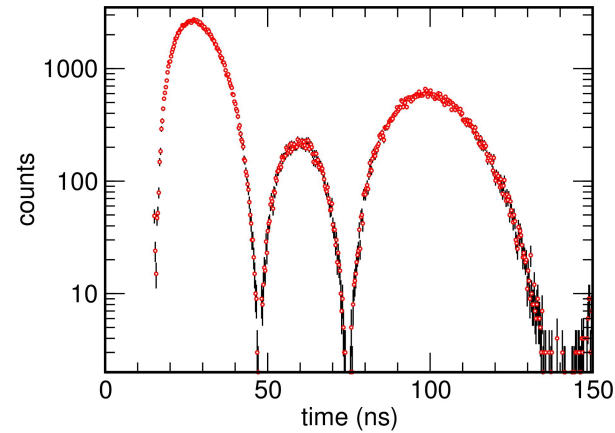


# SMS examples, quadrupole splitting, isomer shift:

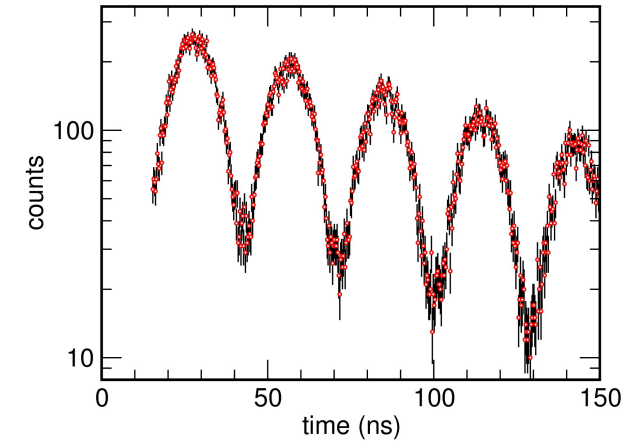
➤ example 2.1  
thickness  $0.1\mu\text{m}$



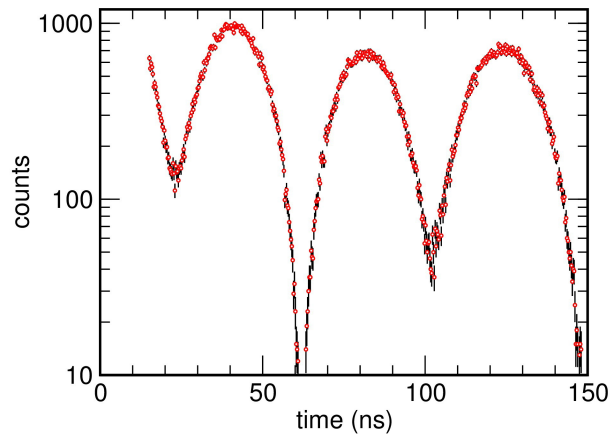
➤ example 2.2



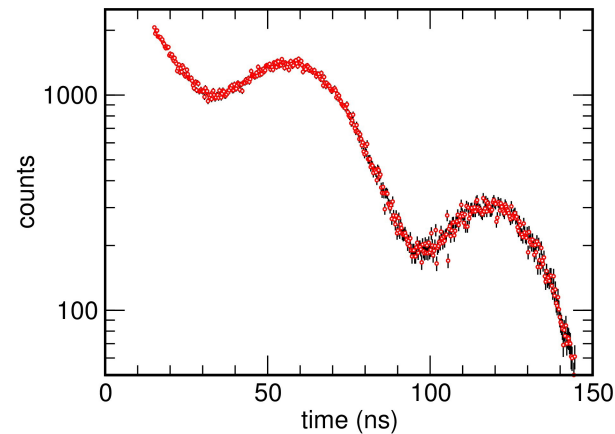
➤ example 2.3  
thickness  $0.1\mu\text{m}$ ; texture



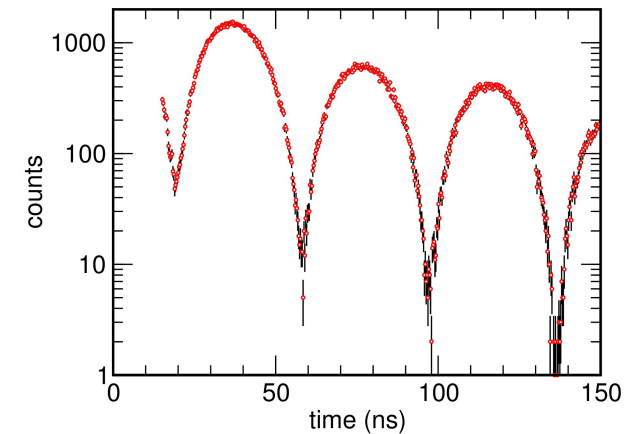
➤ example 3.1  
 $0.1\mu\text{m}$ ; two sites



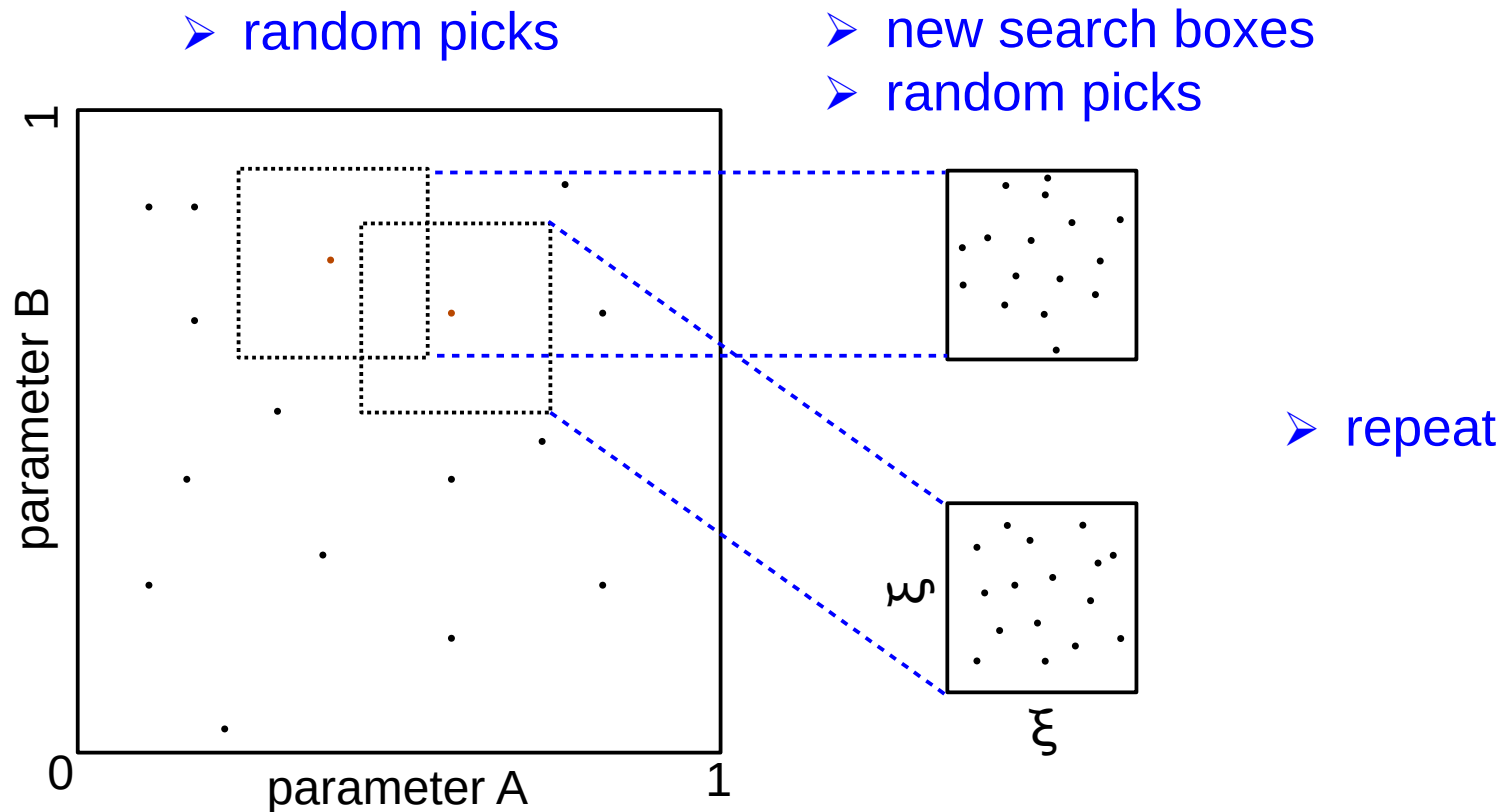
➤ example 3.2  
 $0.1\mu\text{m}$ ; two sites



➤ example 3.3  
 $0.1\mu\text{m}$ ; two sites; distr.

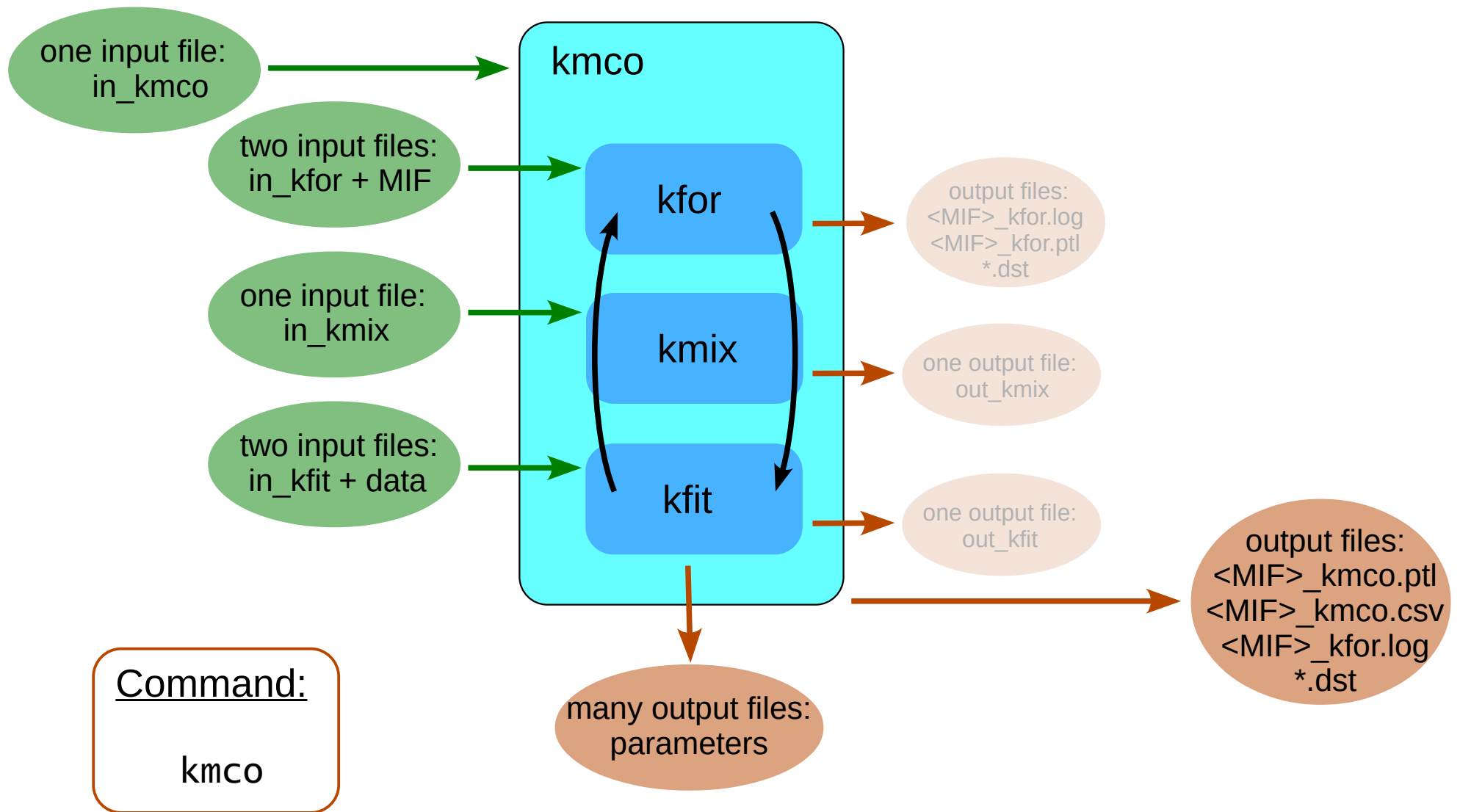


# Randomized search:



☆ in each step the N-dimensional search space shrinks by  $\xi^N$

# Module configuration, Monte Carlo gamble:



# Shotgun approach to fitting of SMS spectra:

## ➤ strategy

- ☆ identify relevant parameters
- ☆ explore parameter space using command `kmco`
- ☆ optimize parameter values using `kctl`

## ➤ re-do examples that you thought most difficult to fit

- ☆ construct the input files `in_kfor`, `in_kmix`, `in_kfit`, `exp.mif`, `in_kctl`
- ☆ focus on isomer shift, thickness, quadrupole splitting

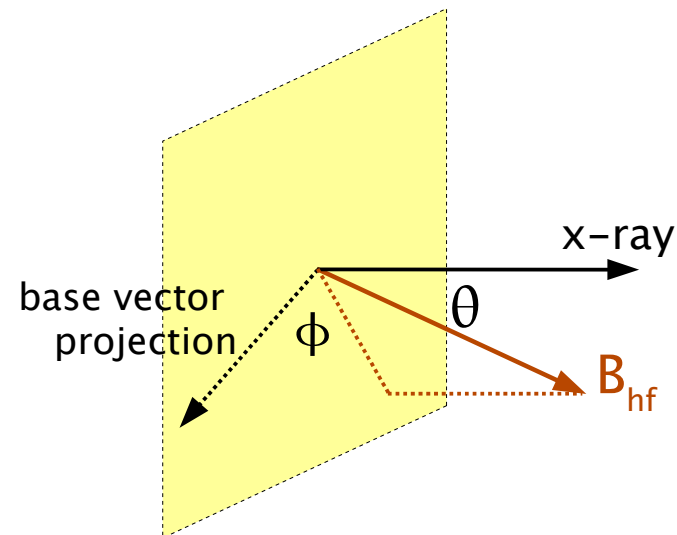
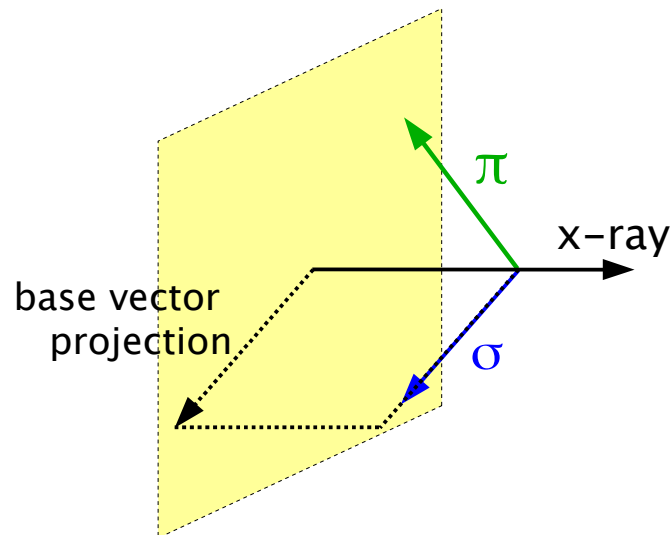
**END OF SATURDAY'S CLASS.**

**TOMORROW: MAGNETIC FIELDS**



# Polarization and magnetic field directions:

- defined by a chosen base vector projection and the direction of the x-rays
- base vector  $(1,0,0)$  is used for the projection unless the x-rays are collinear with  $(1,0,0)$ ; then base vector  $(0,1,0)$  is used for the projection.



# Magnetic SMS spectra:

## ➤ strategy

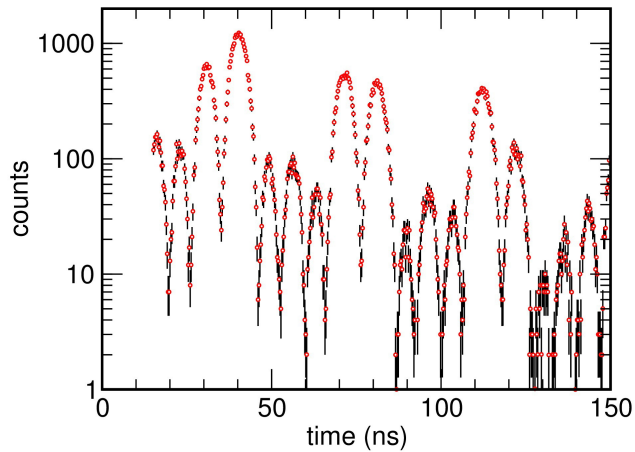
- ☆ identify relevant parameters
- ☆ use your choice approach...

## ➤ examples 4.1-3 and 5.1-3

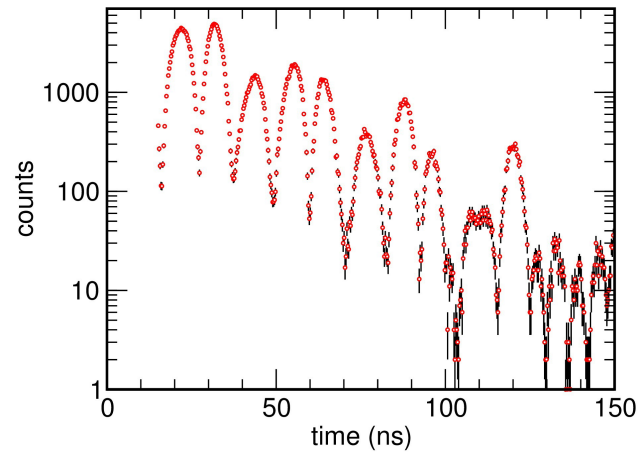
- ☆ construct the input files `in_kfor`, `in_kmix`, `in_kfit`, `exp.mif`, `in_kctl`
- ☆ focus on magnetic fields: magnitude, direction, and distribution

# SMS examples, magnetic fields:

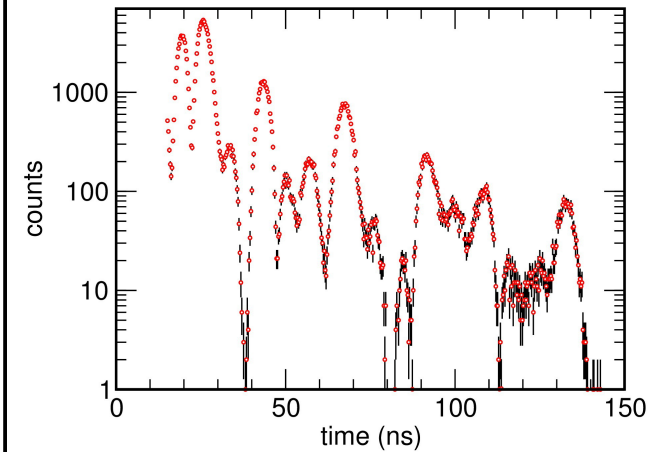
➤ example 4.1  
no texture



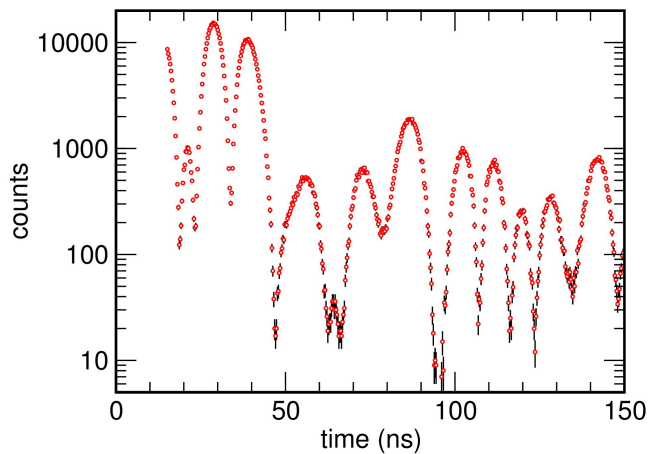
➤ example 4.2  
texture



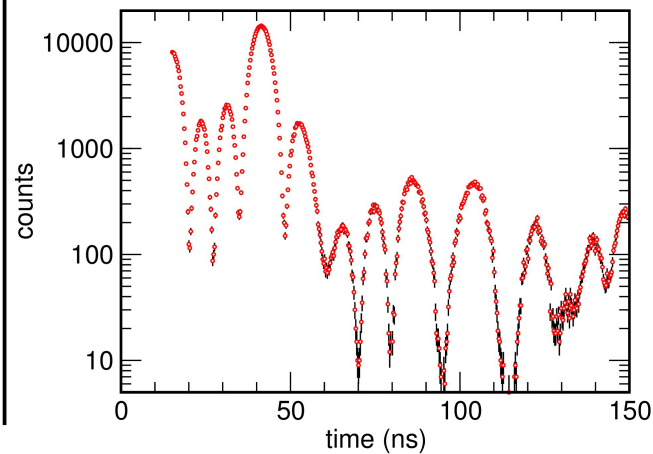
➤ example 4.3  
no texture; distribution



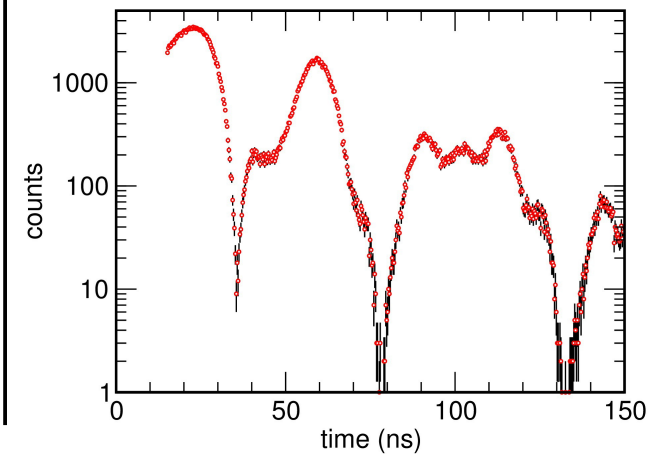
➤ example 5.1  
no texture



➤ example 5.2

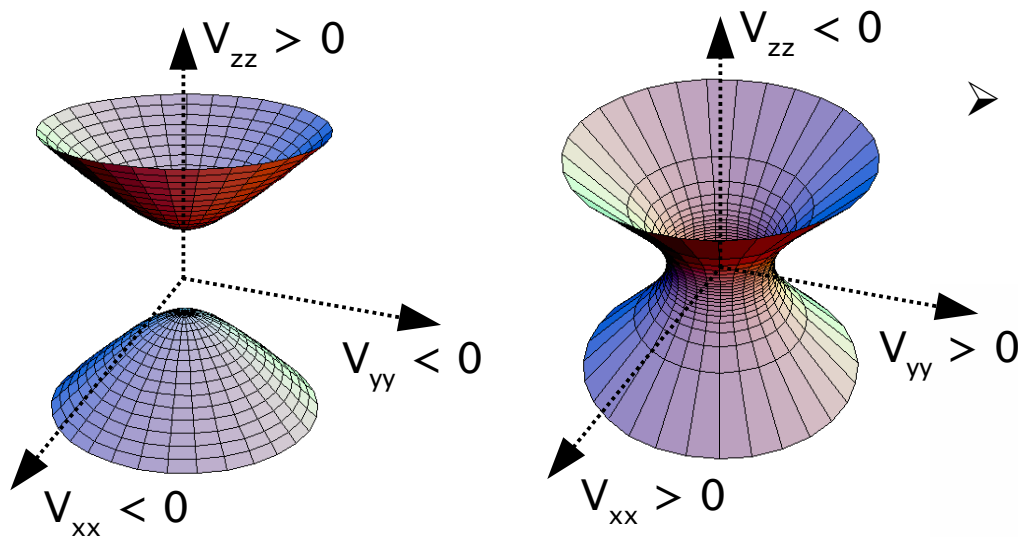


➤ example 5.3

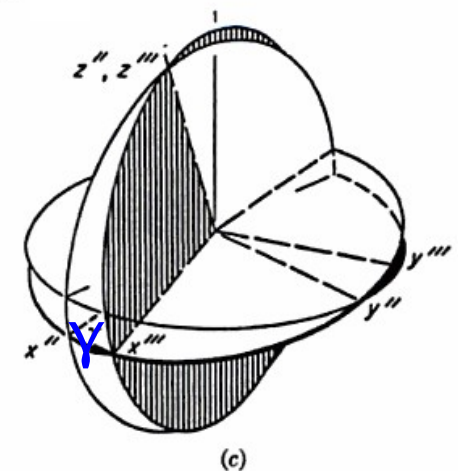
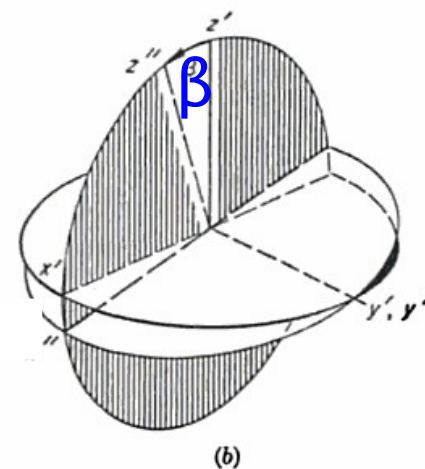
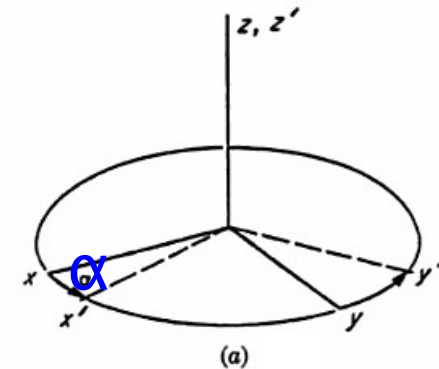


# Electric field gradient as hyperboloid:

- axes:  $|V_{zz}| > |V_{yy}| > |V_{xx}|$   
 $V_{zz} + V_{yy} + V_{xx} = 0$
- asymmetry parameter:  $|V_{yy} - V_{xx}| / |V_{zz}|$



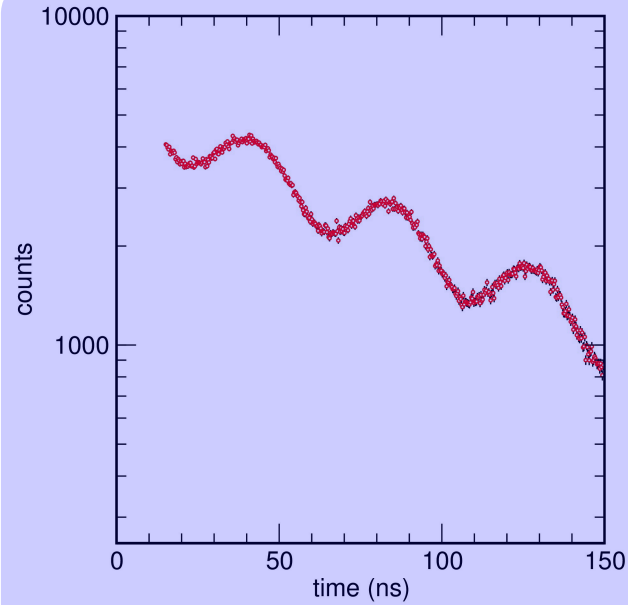
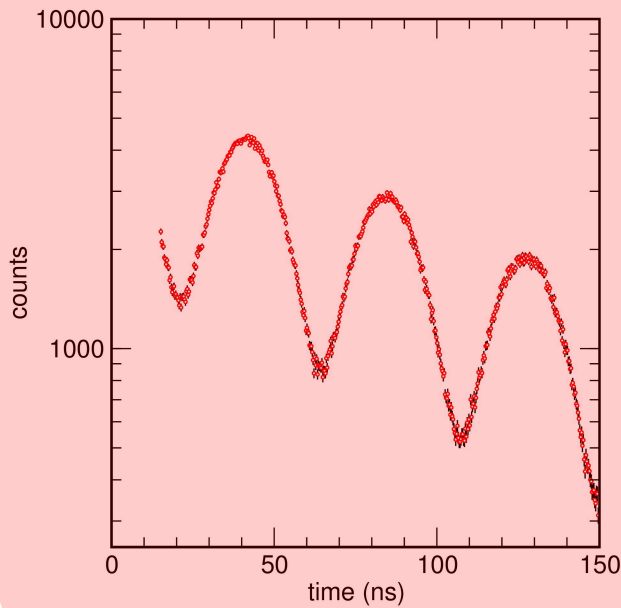
- the orientation is defined by the Euler angles  $(\alpha, \beta, \gamma)$  that rotate the ellipsoid out of the reference frame given by the unit cell.



# SMS examples:

- $V_{zz}$  is perpendicular to the x-ray direction, thickness  $0.1 \mu\text{m}$

➤ example 7.1



➤ example 7.2

➤ example 7.3

