NRIXS software

CONUSS

***CO**herent **NU**clear **S**cattering from **S**ingle crystals*

Software for the evaluation of Synchrotron Mössbauer Spectra

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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)

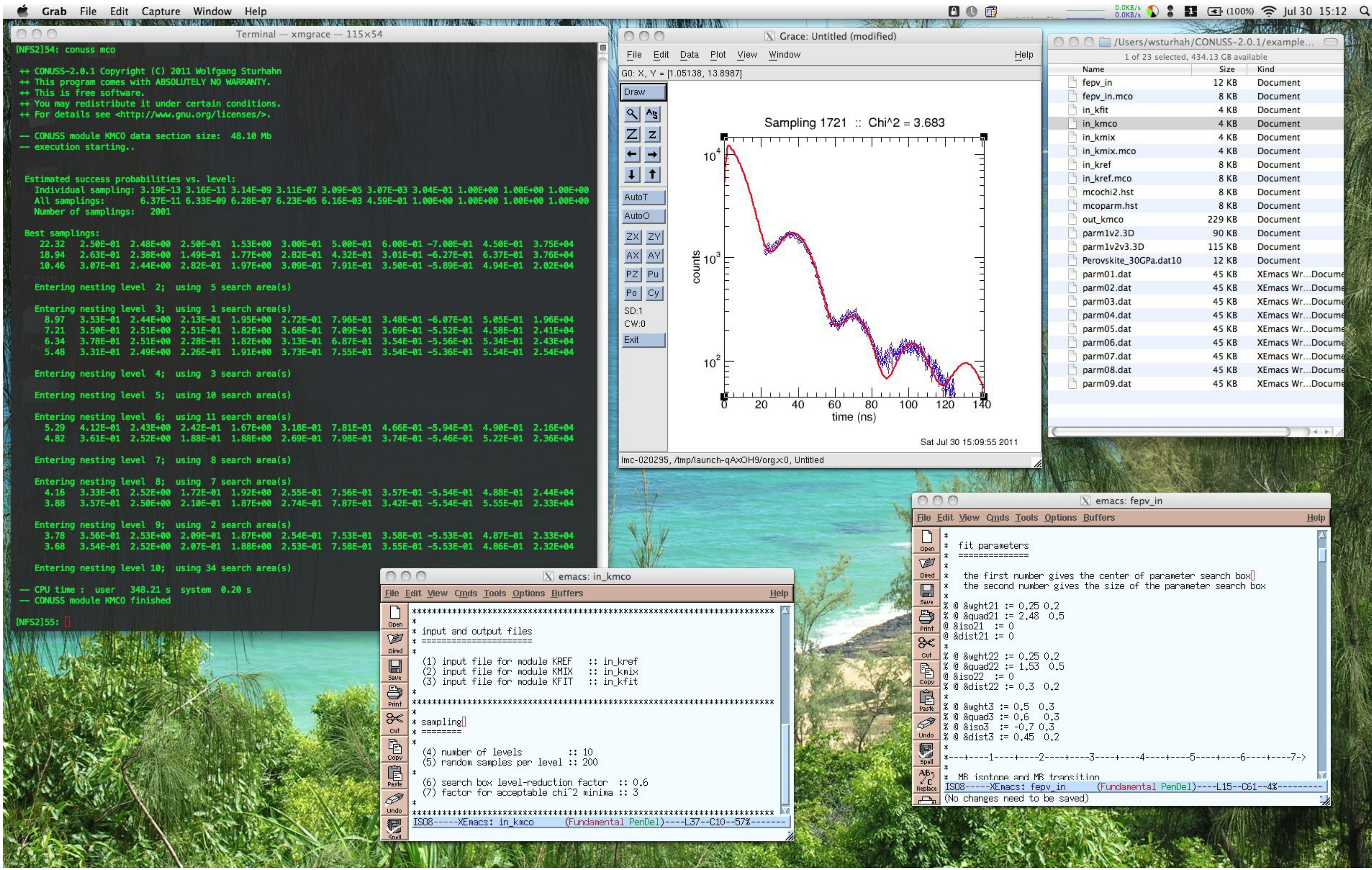
More on CONUSS:

- 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

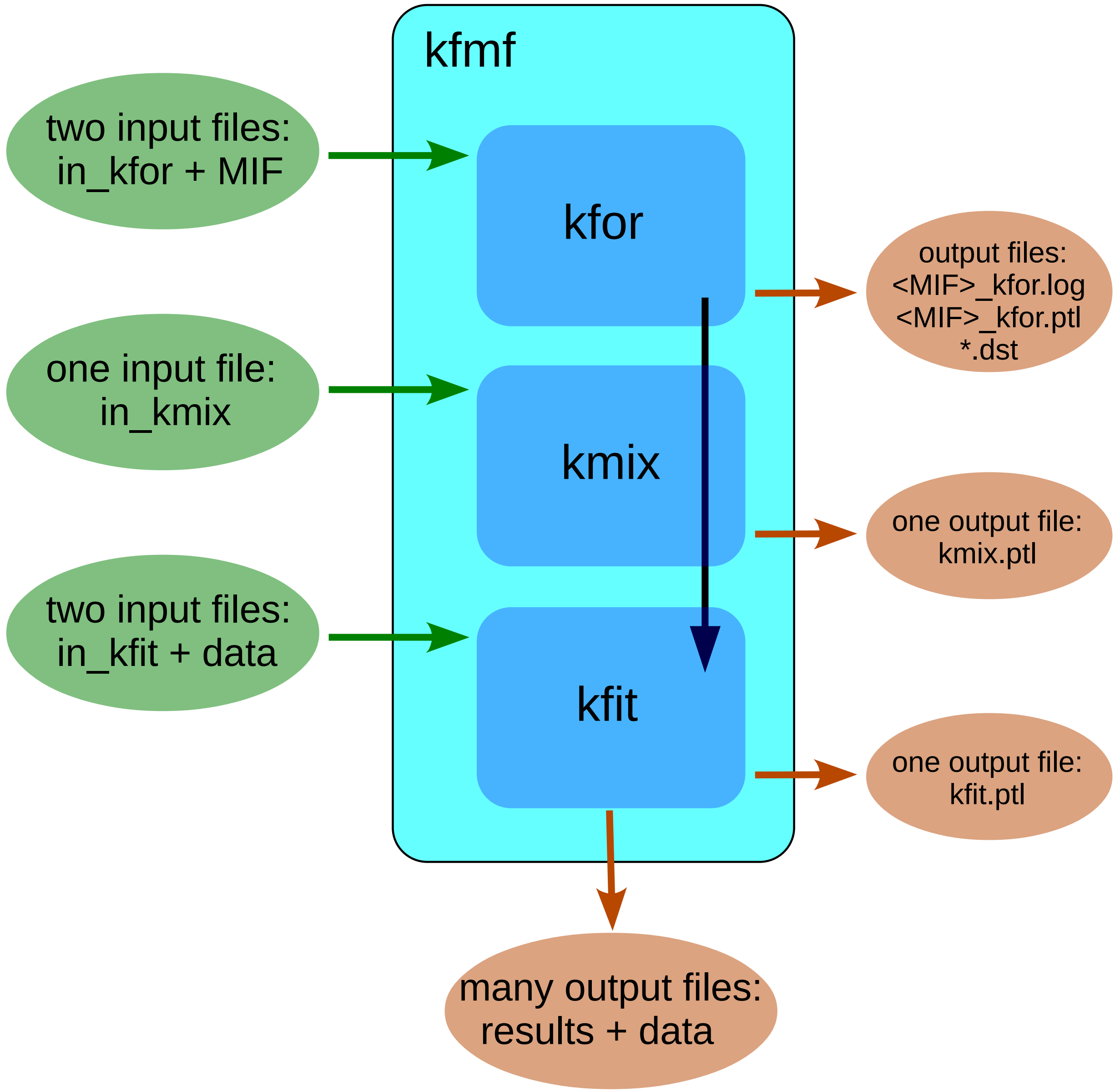
CONUSS now supports:

- 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:



Module configuration, theory and simple fit:



energy-dependent
index-of-refraction

polarization,
Fourier transform

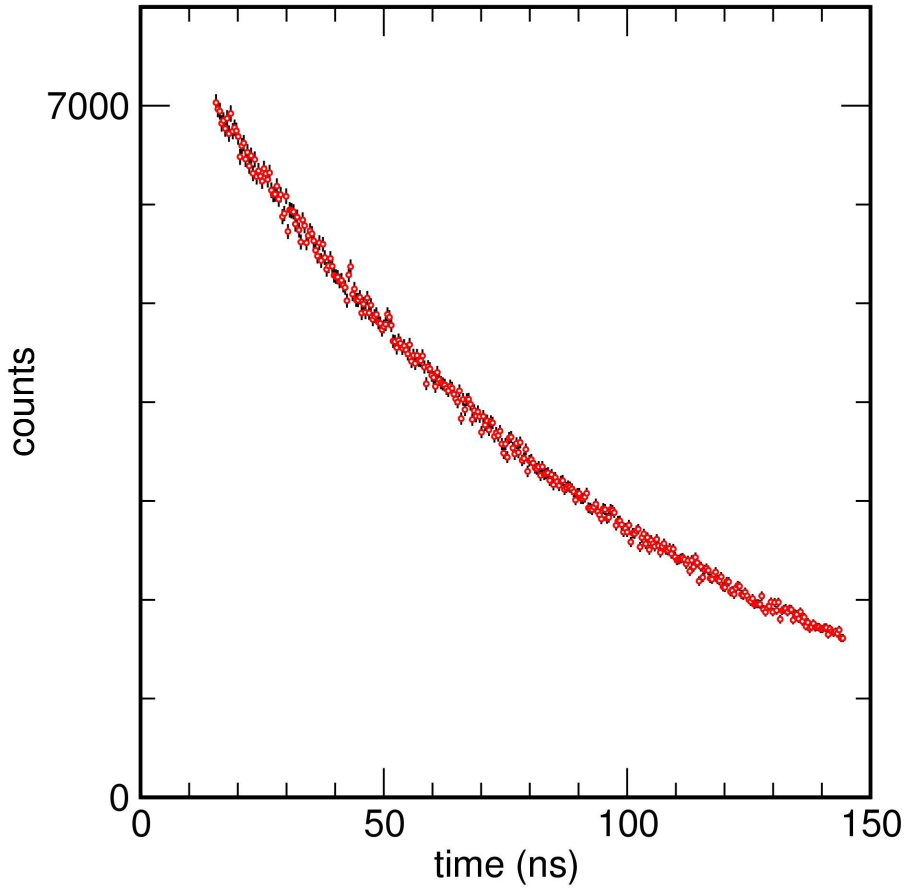
averaging,
comparison to data

Command:

```
kfmf
```

SMS example 1.1:

➢ simulate the following SMS spectrum



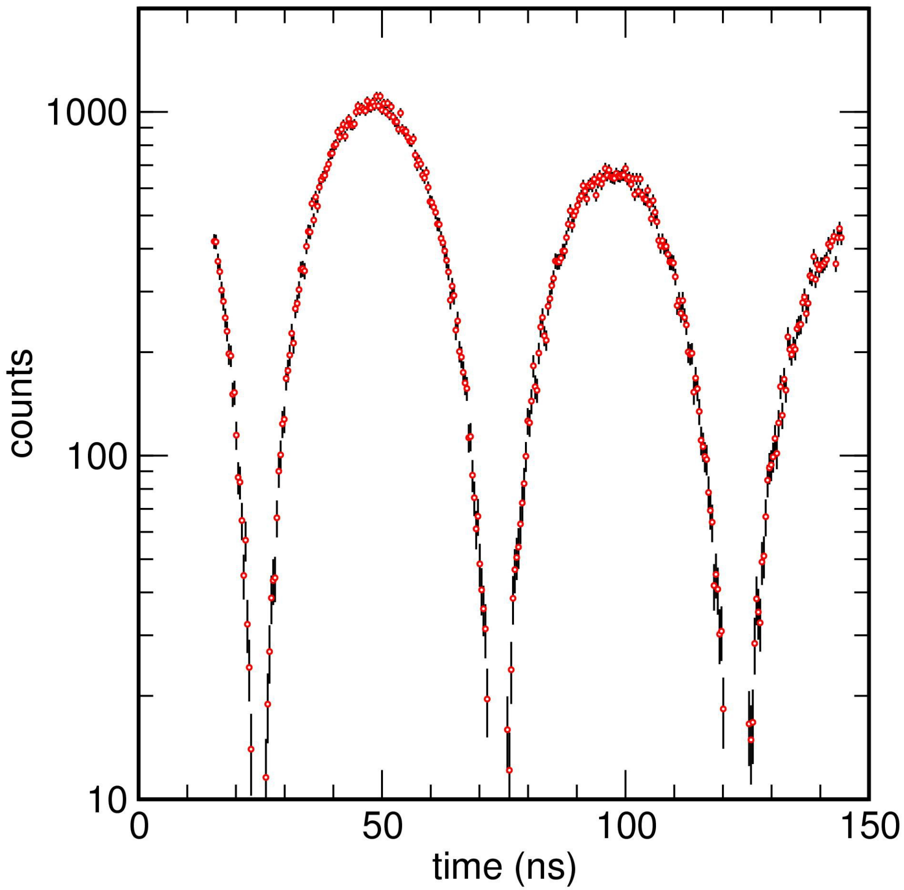
✩ construct the input files
in_kfor, in_kmix, in_kfit, ex1-1.mif

✩ observe the effect of isomer shift,
thickness, quadrupole splitting

✩ Tips: watch correlations

SMS example 2.1:

➢ simulate the following SMS spectrum

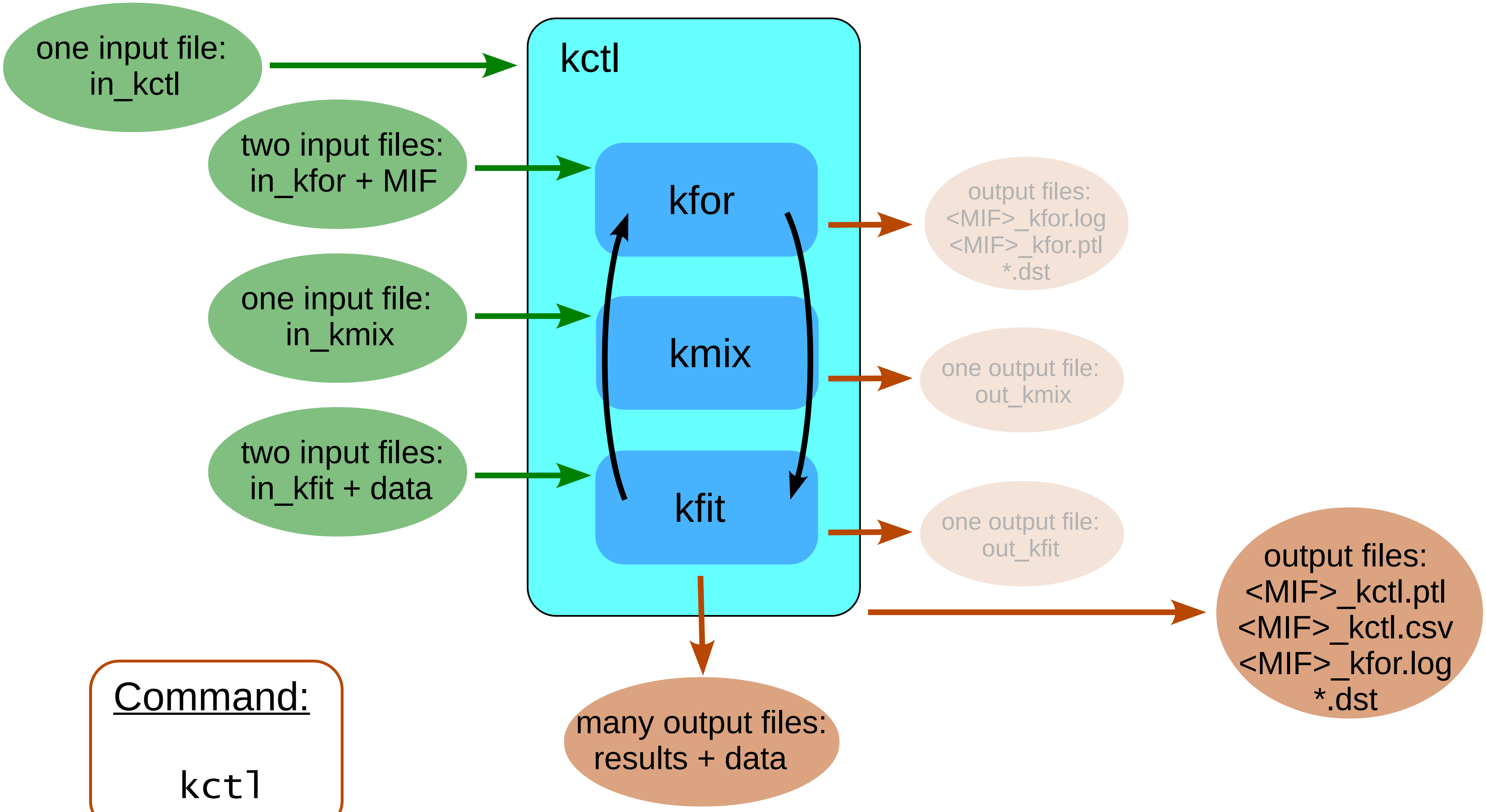


✫ construct the input files
in_kfor, in_kmix, in_kfit, ex2-1.mif

✫ observe the effect of thickness,
quadrupole splitting

✫ Tips: watch correlations

Module configuration, general fitting:



Command:

```
kctl
```

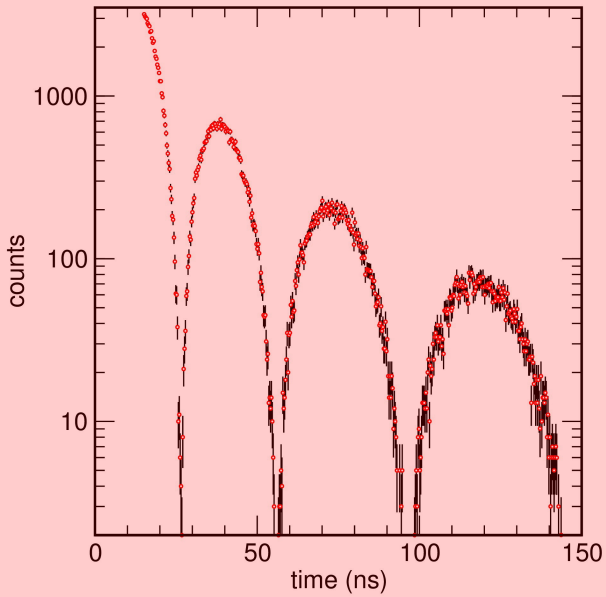
Fitting of SMS spectra:

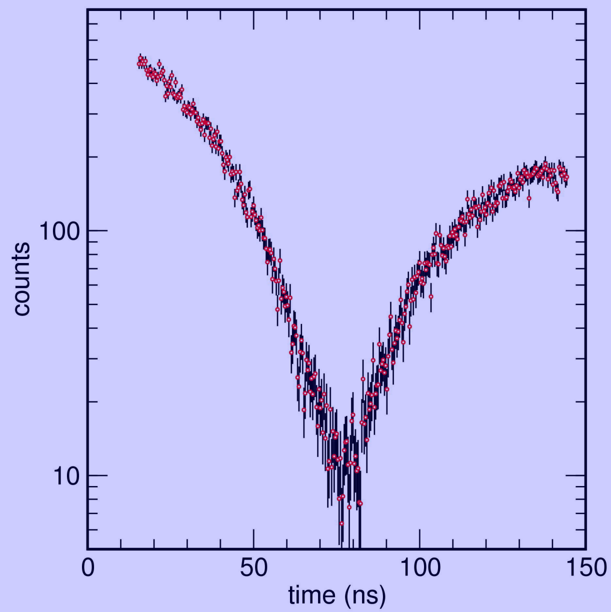
- strategy
  - identify relevant parameters
  - find start values using command `kfmf`
  - optimize parameter values using `kctl`

- 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:

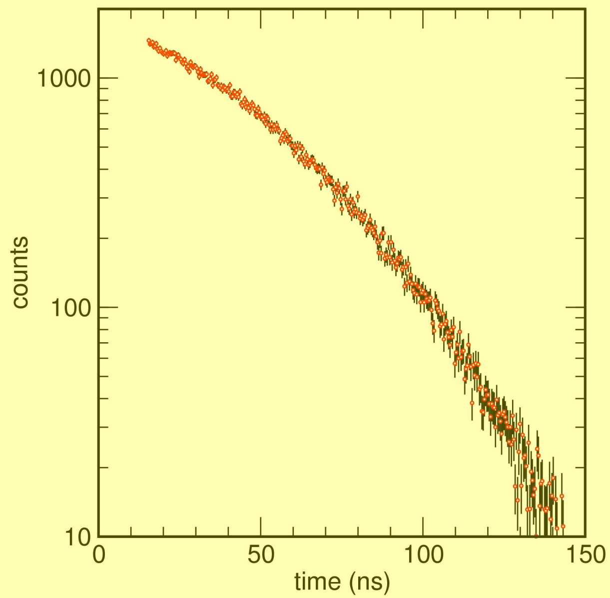
➢ example 1.2
focus on thickness





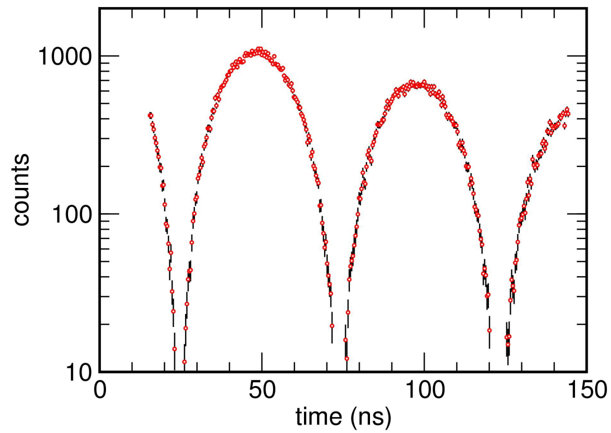
➢ example 1.3
two sites; isomer shift;
thickness 0.1μm

➢ example 1.4
IS distribution;
thickness 0.1μm

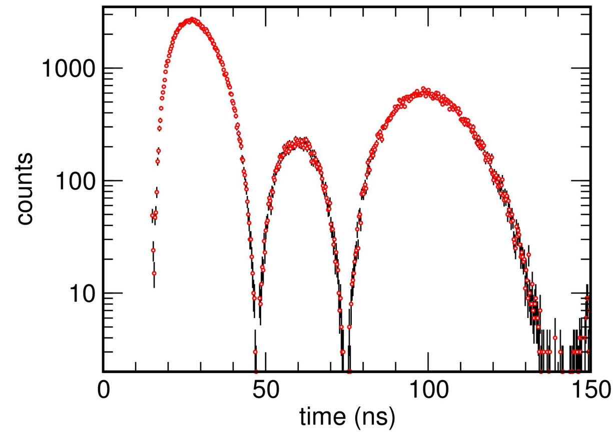


SMS examples, quadrupole splitting, isomer shift:

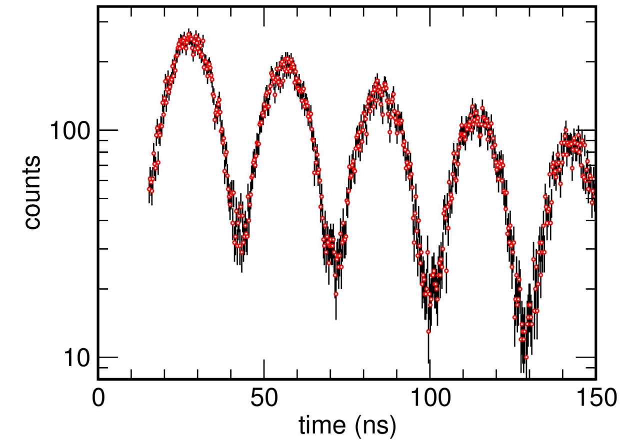
- example 2.1
  thickness 0.1µm



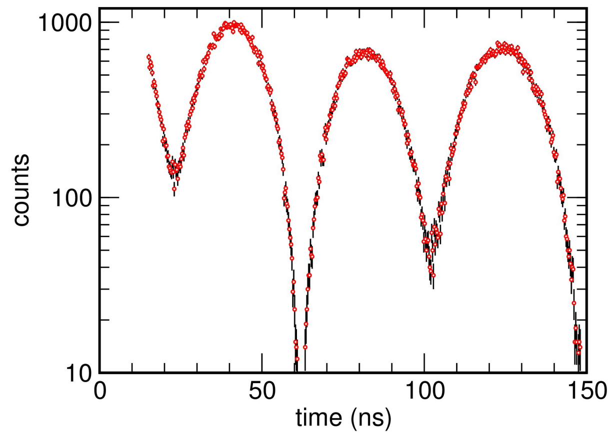
- example 2.2



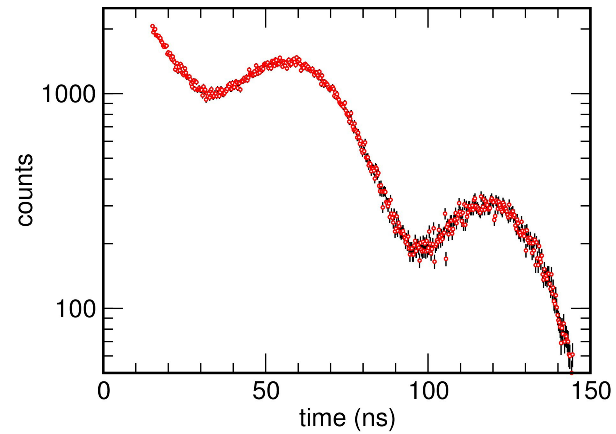
- example 2.3
  thickness 0.1µm; texture



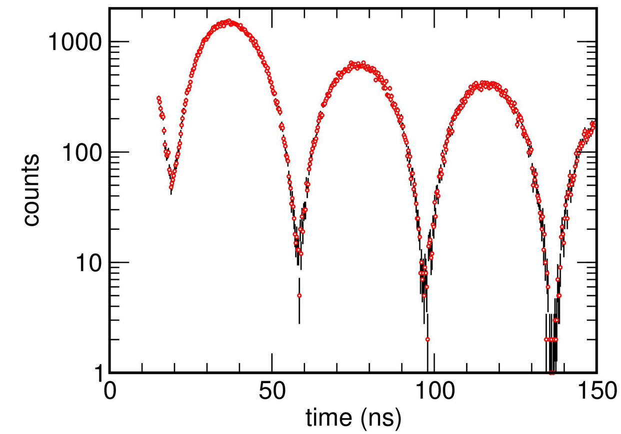
- example 3.1
  0.1µm; two sites



- example 3.2
  0.1µm; two sites

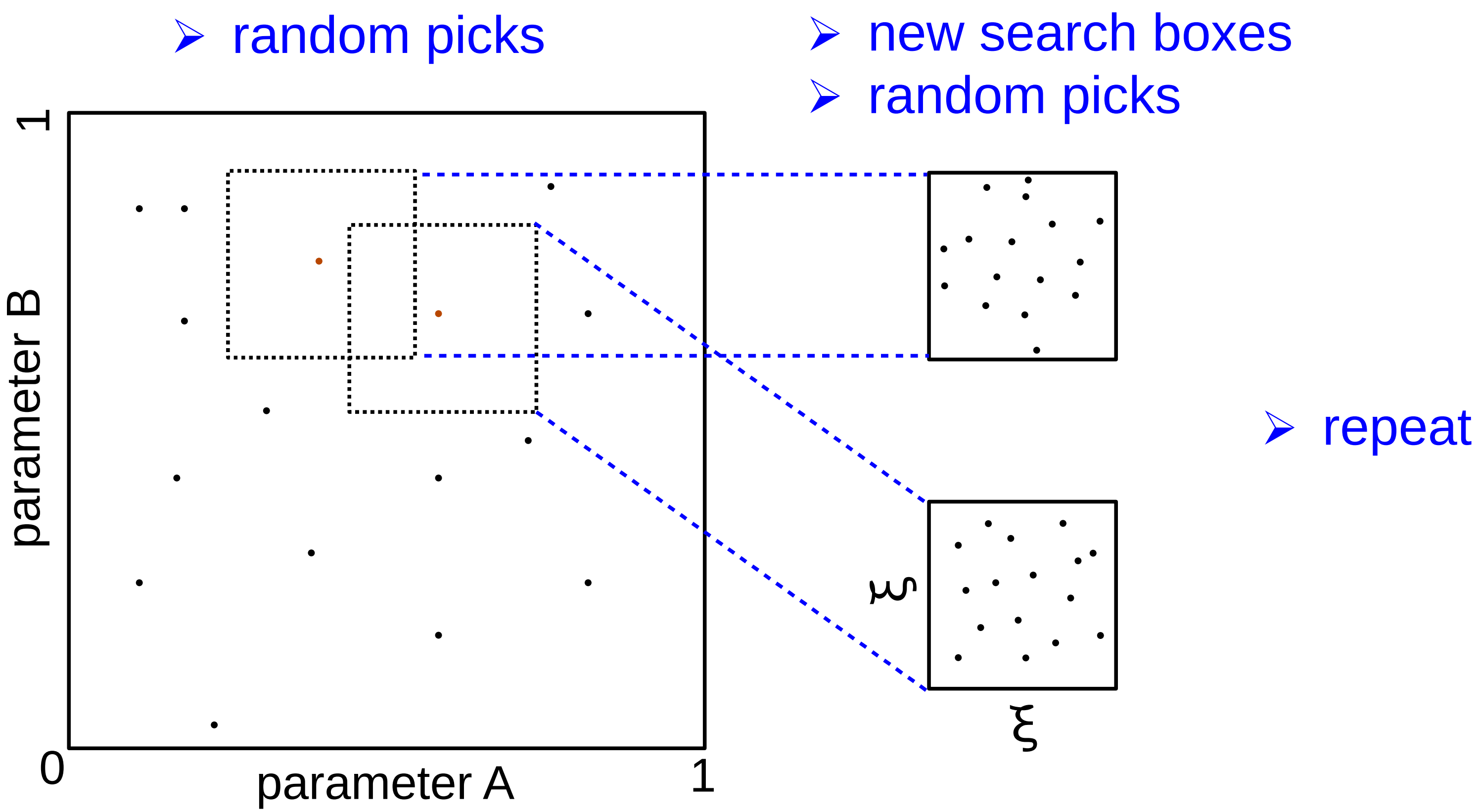


- example 3.3
  0.1µm; two sites; distr.



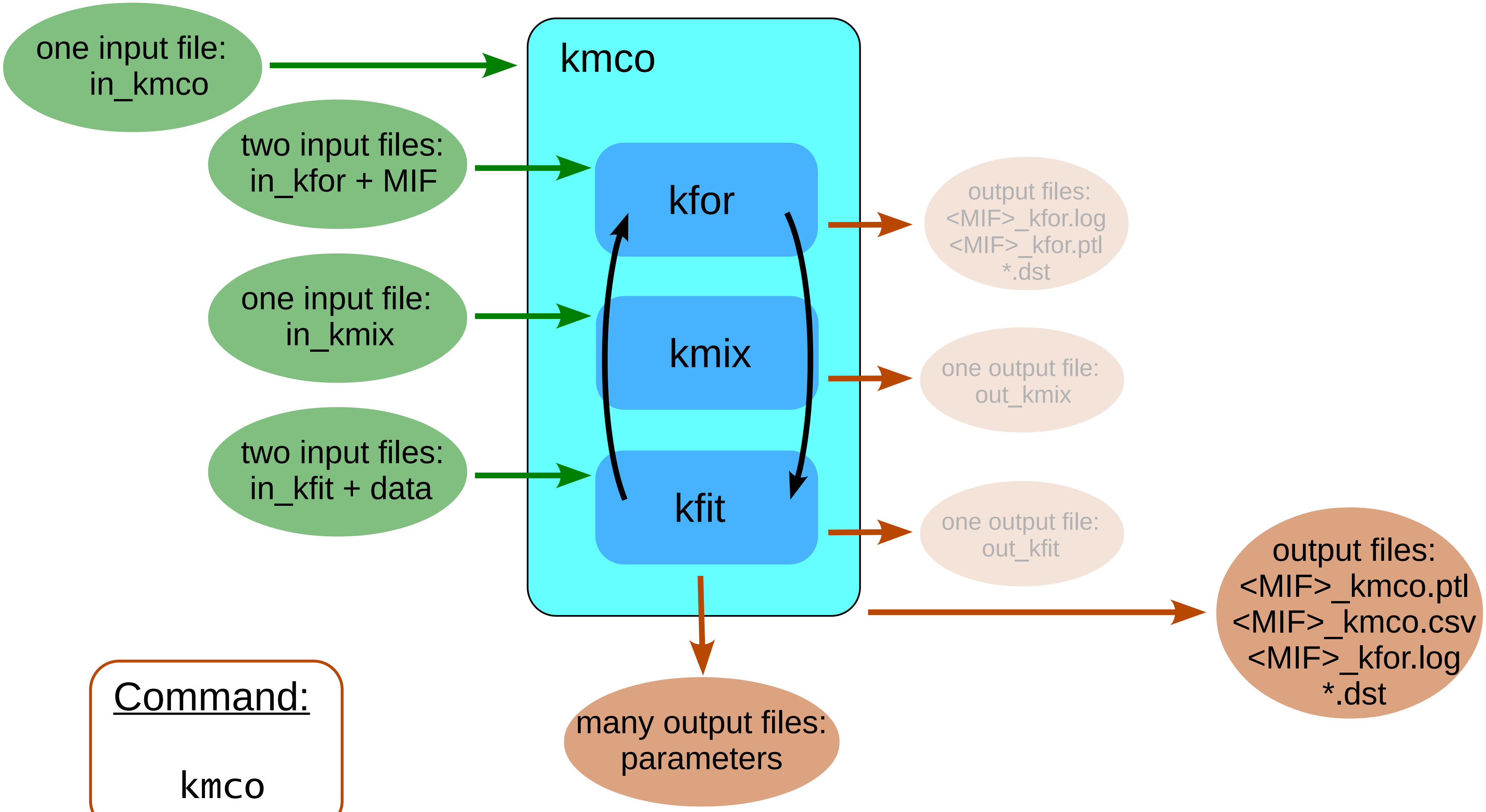
NRIXS software

Randomized search:



☆ in each step the N-dimensional search space shrinks by ξ^N

Module configuration, Monte Carlo gamble:



Command:

`kmco`

Shot gun 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

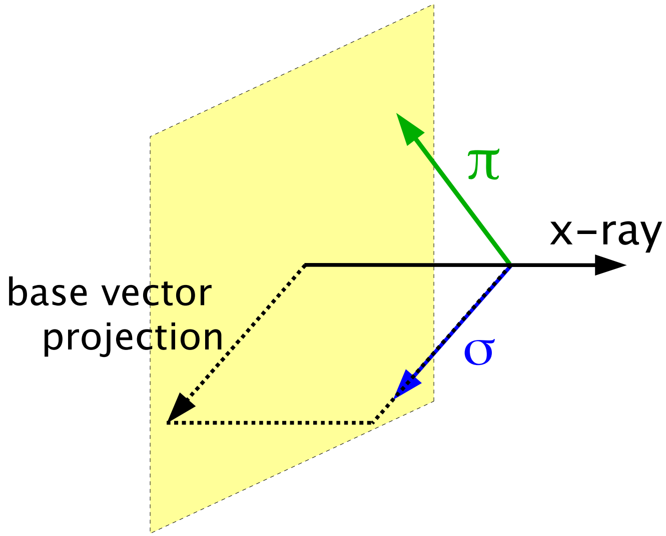
End of Saturday's Class.

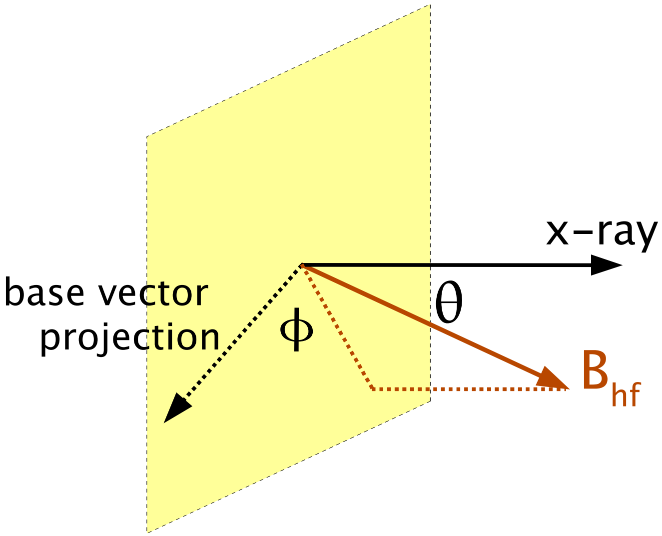
Tomorrow: Magnetic Fields

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.





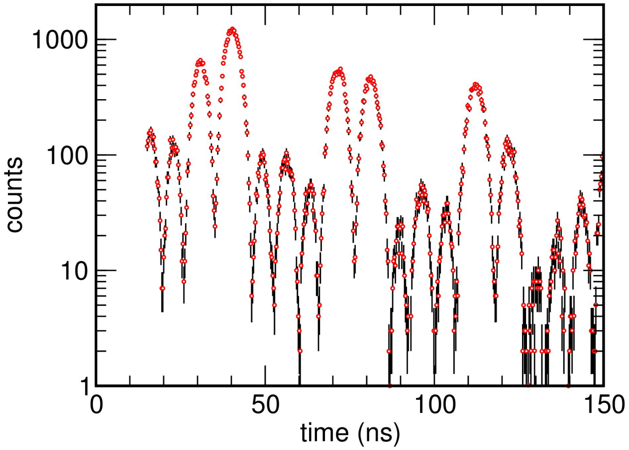
Magnetic SMS spectra:

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

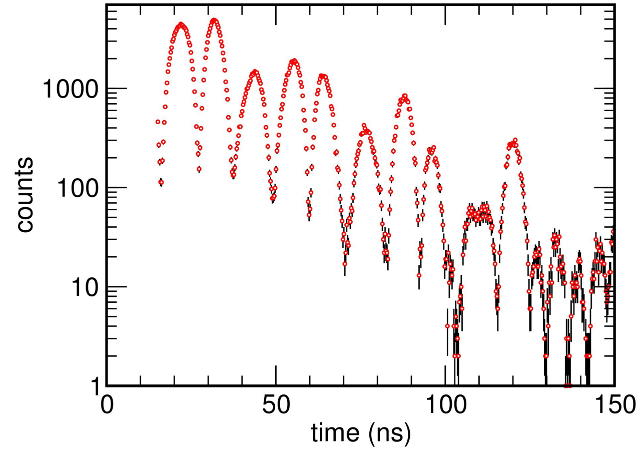
- examples 4.1-3 and 5.1-3
  - construct the input files in_kfor, in_kmix, in_kfit, exp.mif, in_kctl
  - focus on magnetic fields: magnitude, direction, and distribution

SMS examples, magnetic fields:

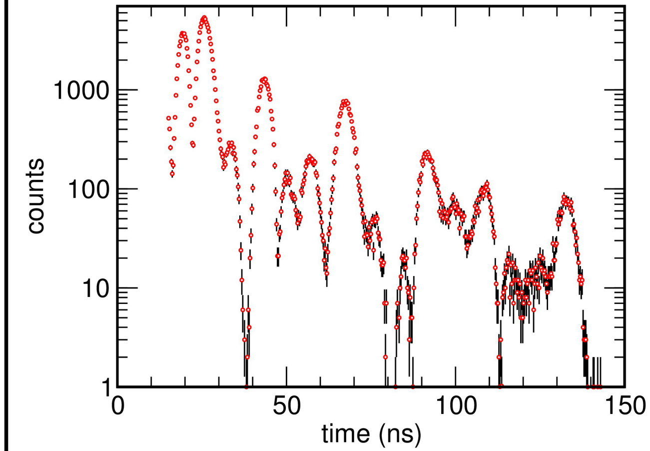
- example 4.1
  no texture



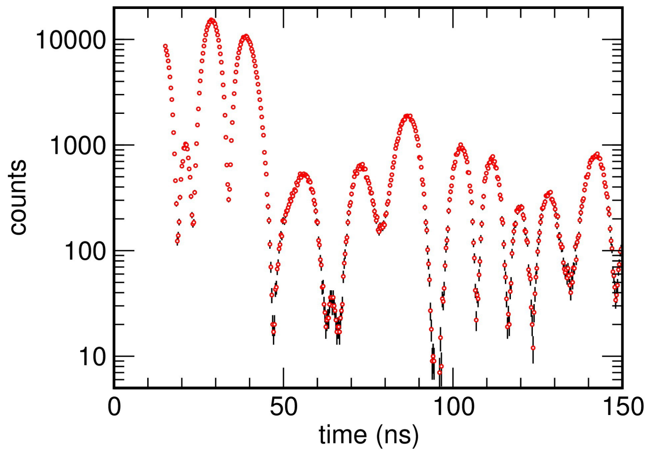
- example 4.2
  texture



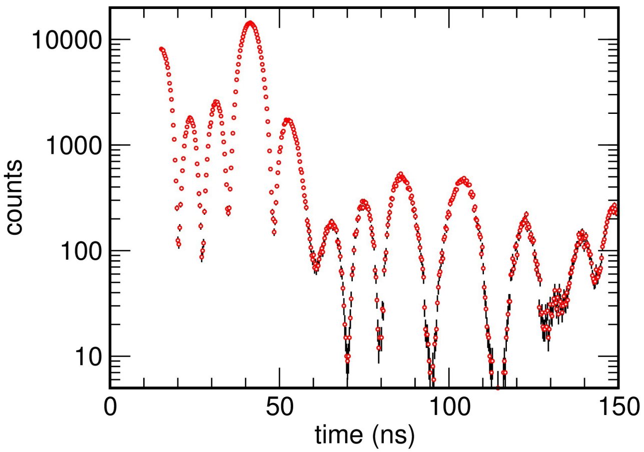
- example 4.3
  no texture; distribution



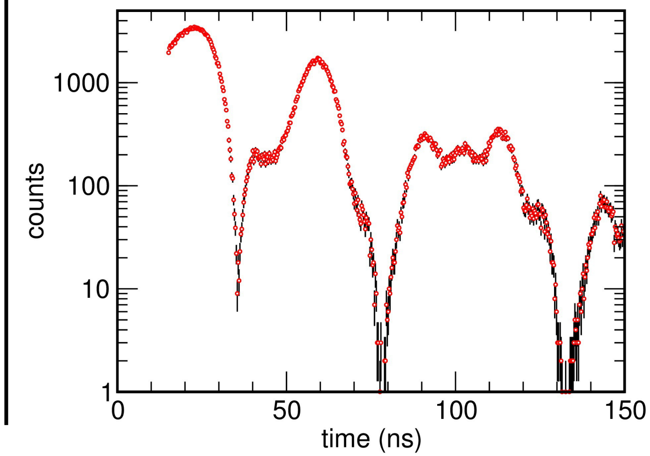
- example 5.1
  no texture



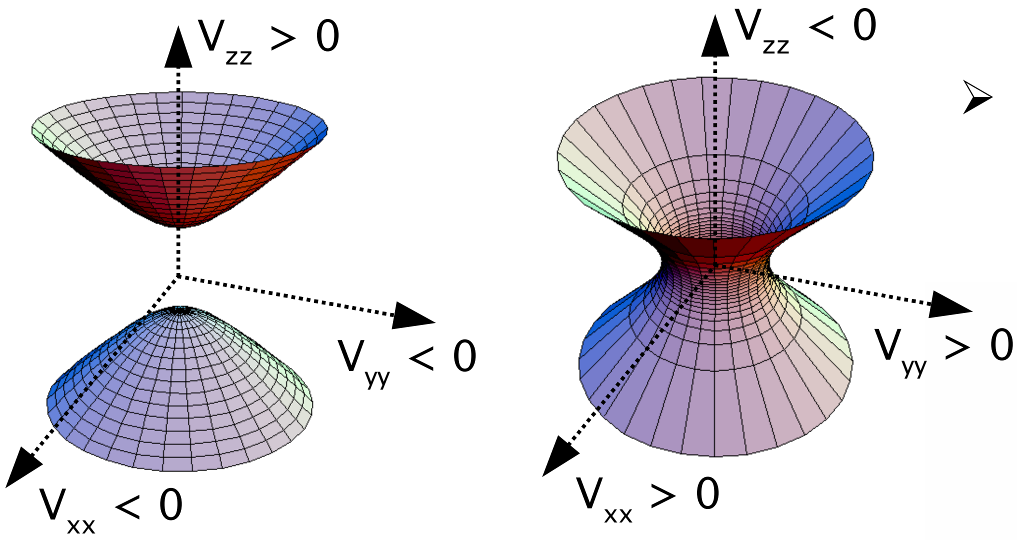
- example 5.2



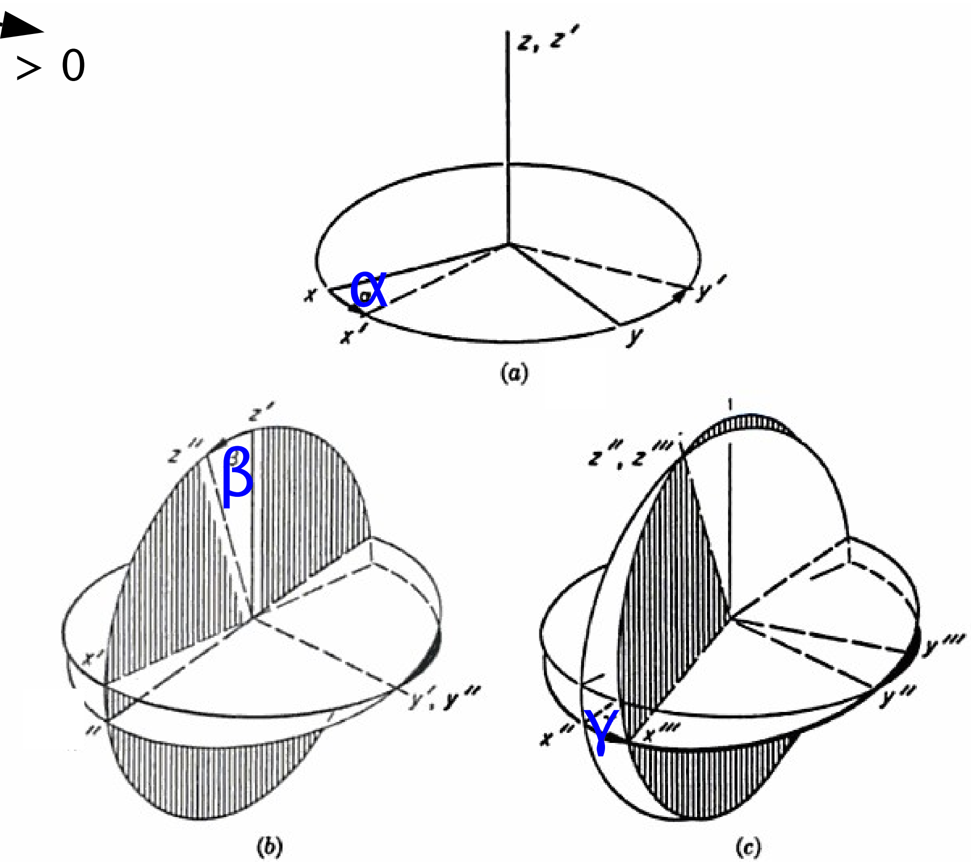
- example 5.3



Electric field gradient as hyperboloid:



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

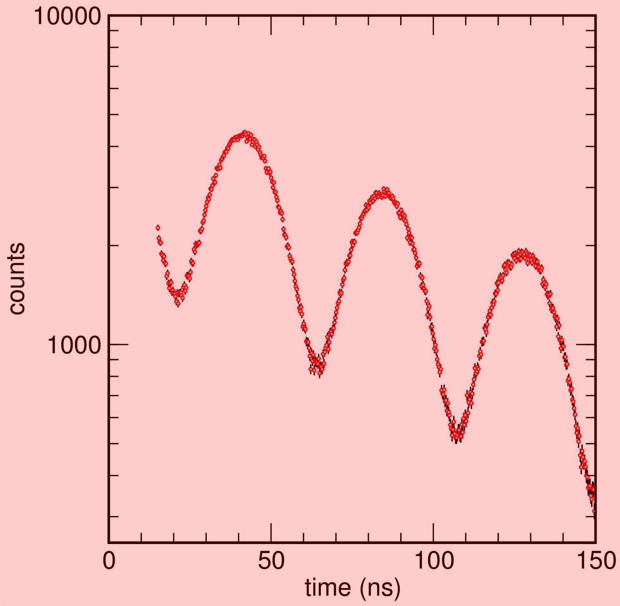


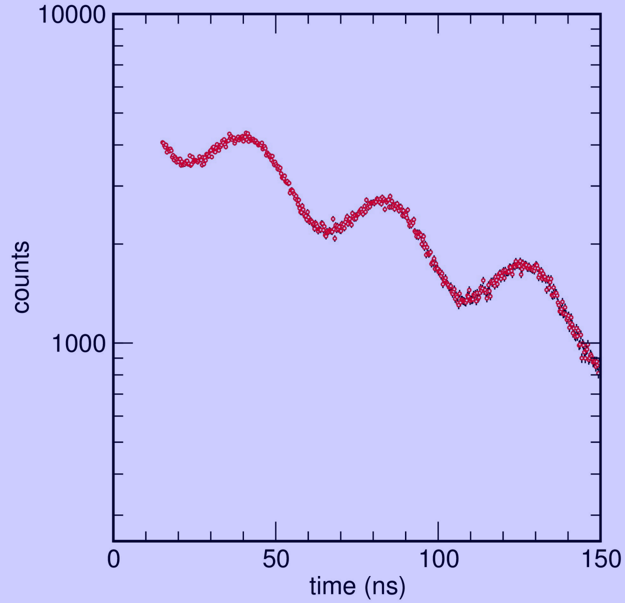
- the orientation is defined by the Euler angles (α,β,γ) that rotate the ellipsoid out of the reference frame given by the unit cell.

SMS examples:

- V_{zz} is perpendicular to the x-ray direction, thickness 0.1 μm

- example 7.1





- example 7.2

- example 7.3