NRIXS software

COherent NUclear Scattering from Single 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 at
  the University of Hamburg (1986-1993)
  the ESRF (1992)
  the APS (1992-2010)
  - ☆ 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

publications related to CONUSS:

W. Sturhahn and E. Gerdau, Phys. Rev. B 49 (1994)
W. Sturhahn, Hyperfine Interact 125 (2000)

CONUSS now supports:

- all Mössbauer isotopes

- forward scattering 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

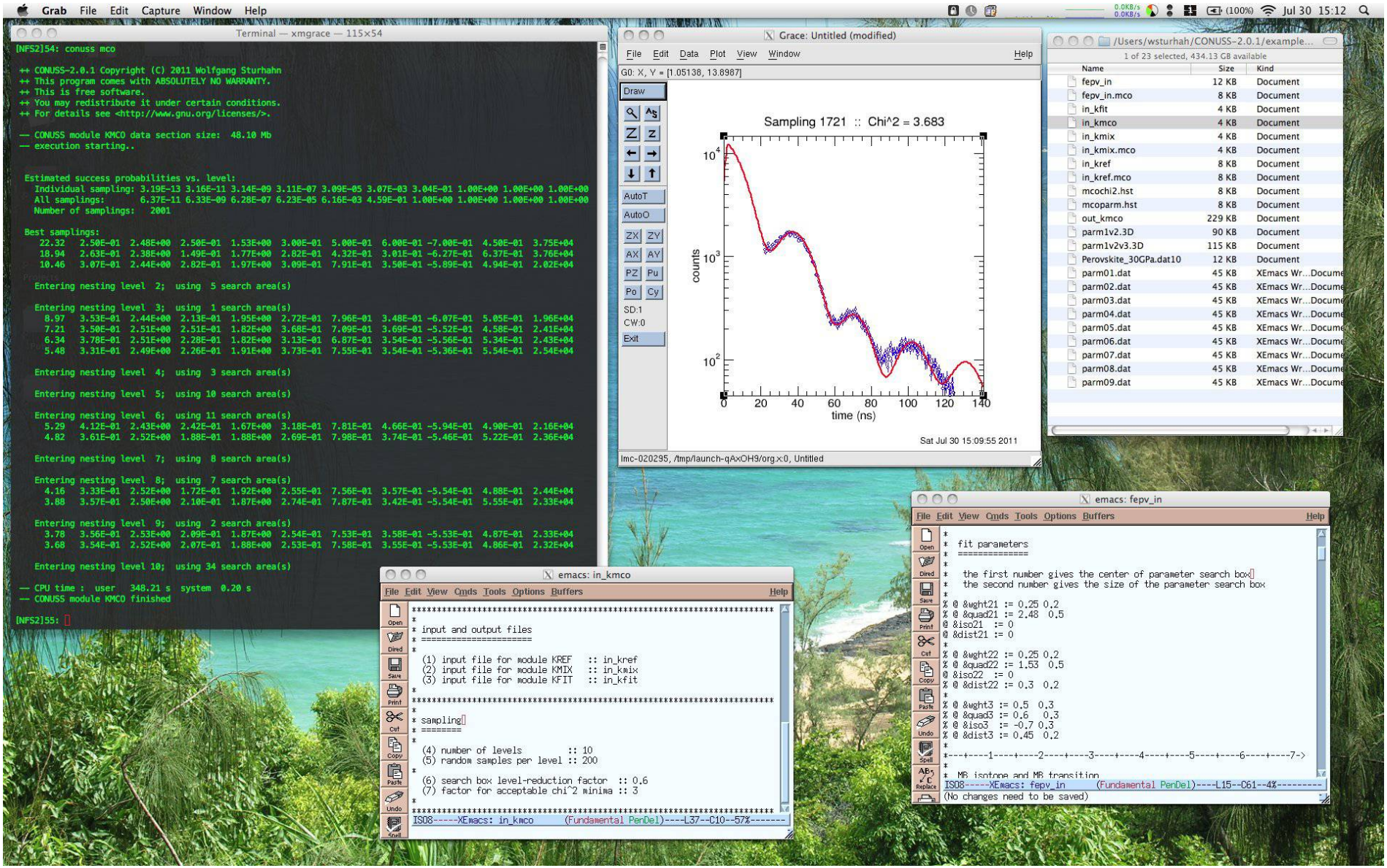
More on CONUSS:

- has been used for data evaluation in numerous publications
- distributed under GPL, source code public, evaluations traceable
- can be obtained per e-mail from Wolfgang Sturhahn, no charge
- a major upgrade, CONUSS-2.0.0, was released in 2010

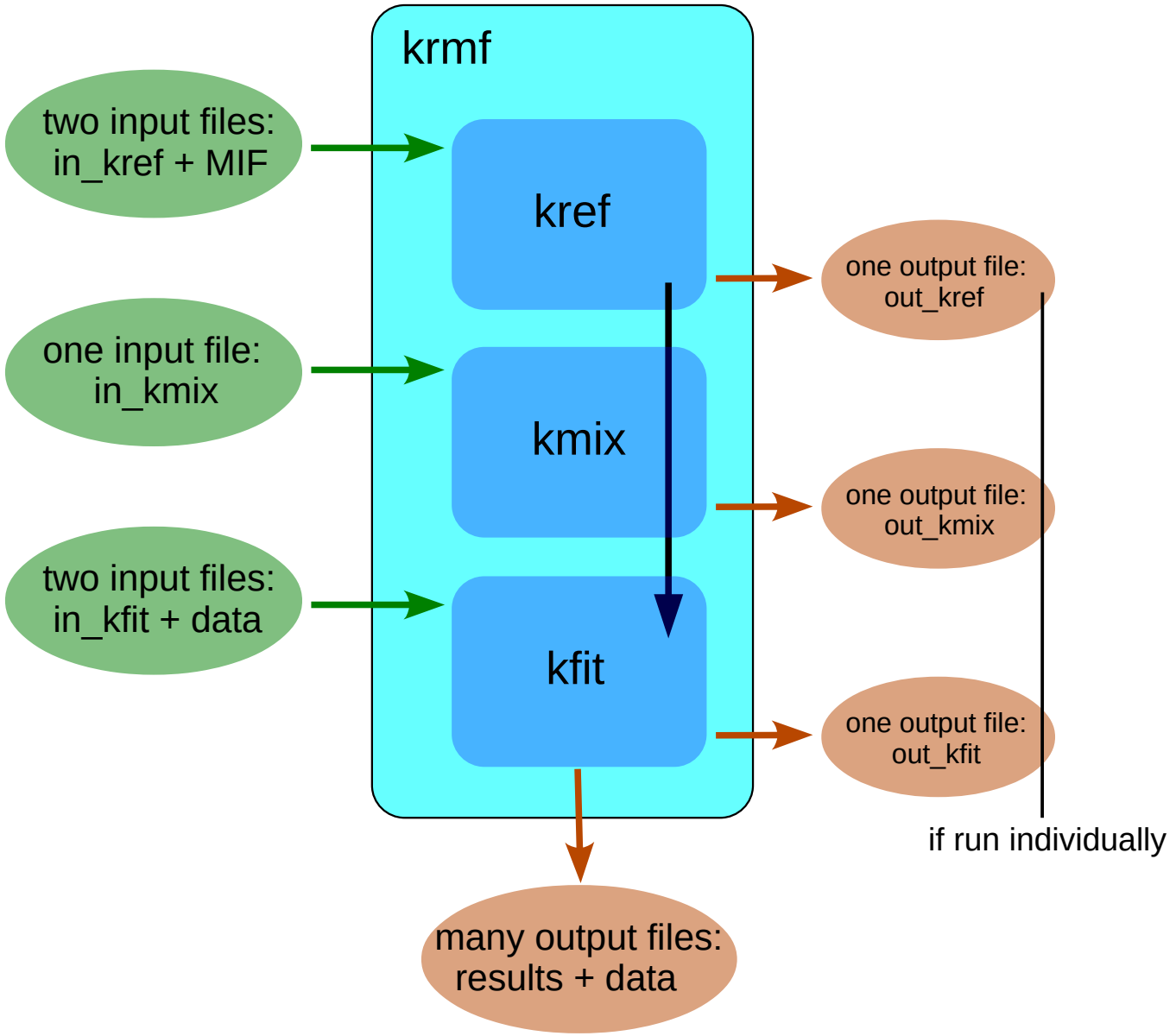
- CONUSS-2.0.0
  - ☆ has a simple installation procedure for Unix and Mac OS X
  - ☆ offers all previous capabilities of CONUSS
  - ☆ has enhanced fit capabilities
  - ☆ features run-time graphics
  - ☆ has a new Monte Carlo approach to find start-values, explore the parameter space, and smart parameter optimization

- possible future development
  - ☆ Graphical input file editor
  - ☆ support of grazing incidence geometry

KMCO app screen shot:



Module configuration, theory and simple fit:



energy-dependent
index-of-refraction

polarization,
Fourier transform

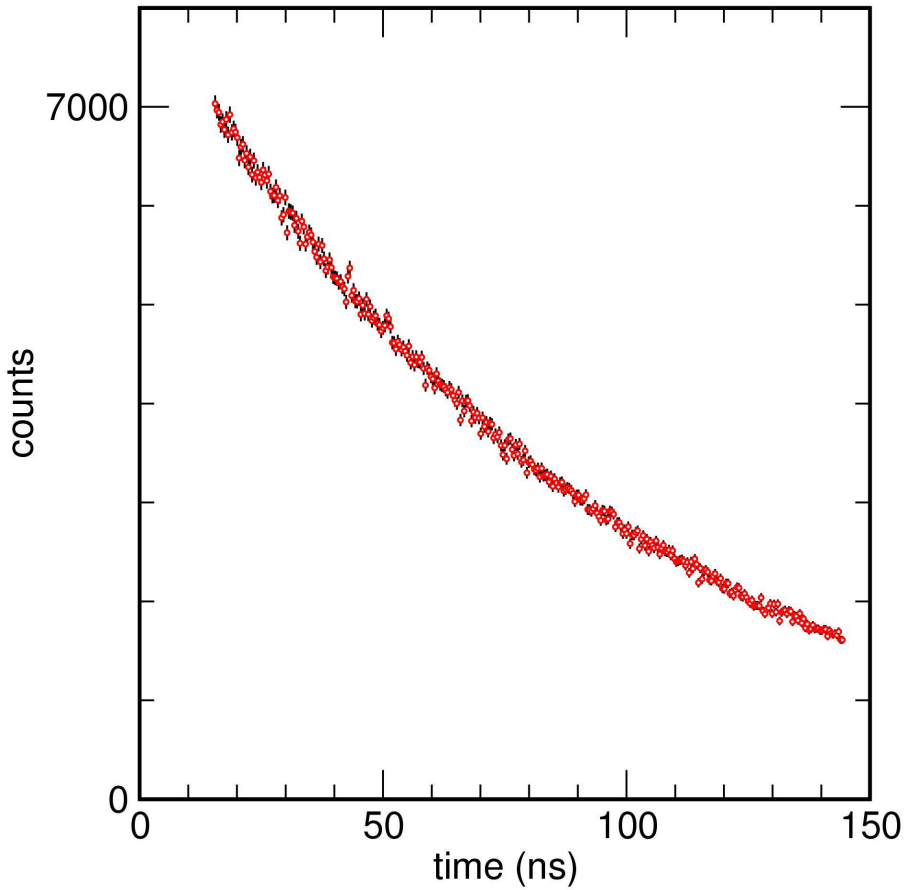
averaging,
comparison to data

Command:

`krmf`

SMS example 1.1:

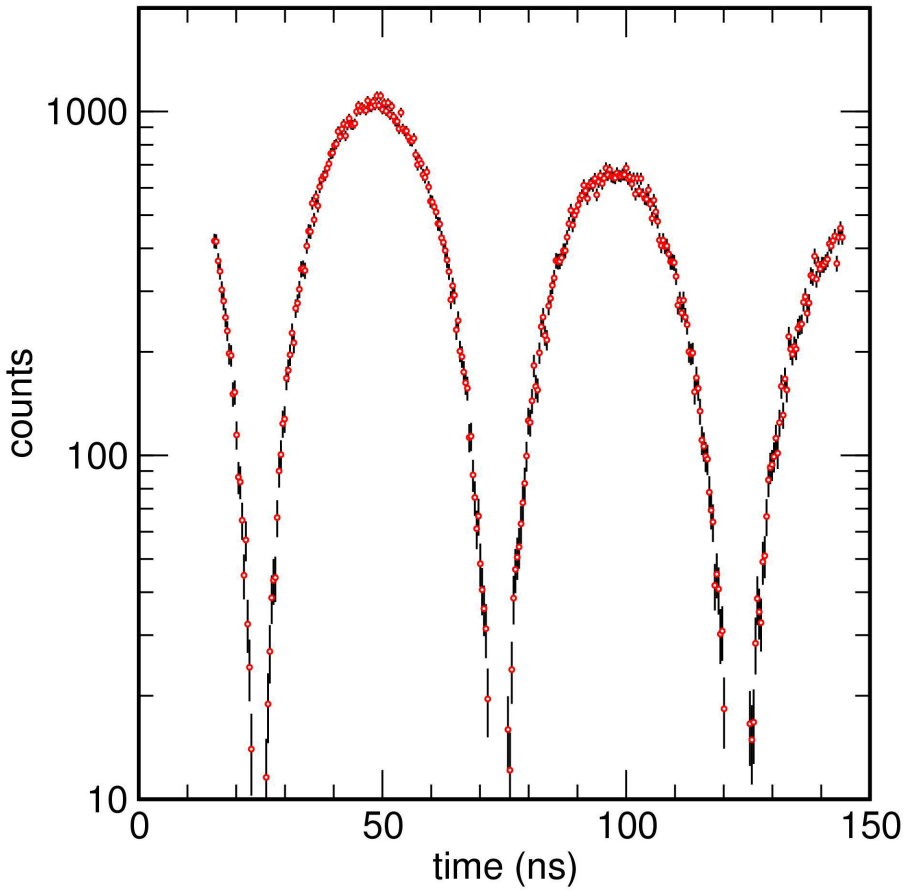
- simulate the following SMS spectrum



- ☆ construct the input files
  in_kref, in_kmix, in_kfit, ex1.1_in
- ☆ observe the effect of isomer shift, thickness, quadrupole splitting
- ☆ Tips: watch correlations

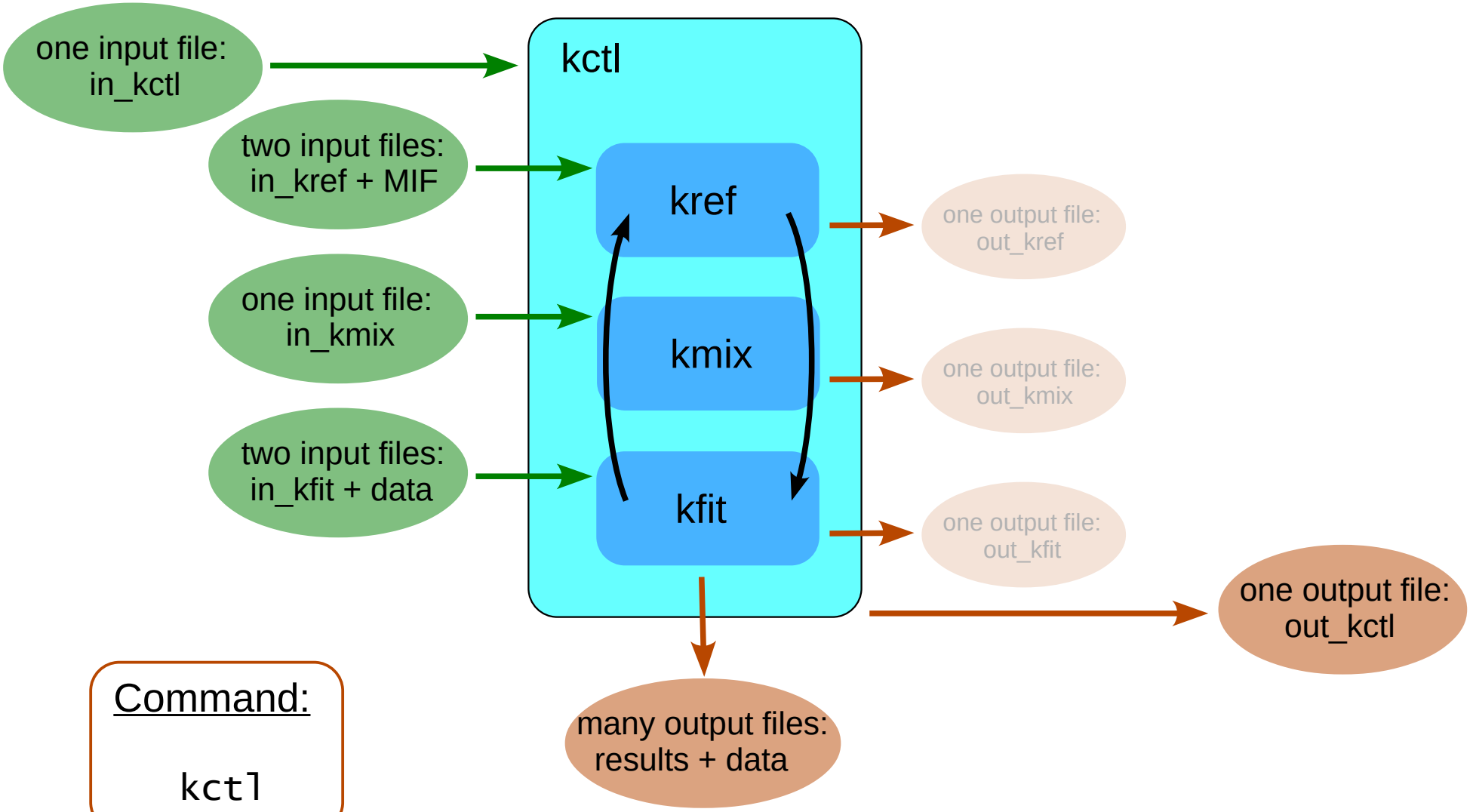
SMS example 2.1:

- simulate the following SMS spectrum



- ☆ construct the input files
  in_kref, in_kmix, in_kfit, ex2.1_in
- ☆ observe the effect of thickness, quadrupole splitting
- ☆ Tips: watch correlations

Module configuration, general fitting:



Command:

```
kctl
```

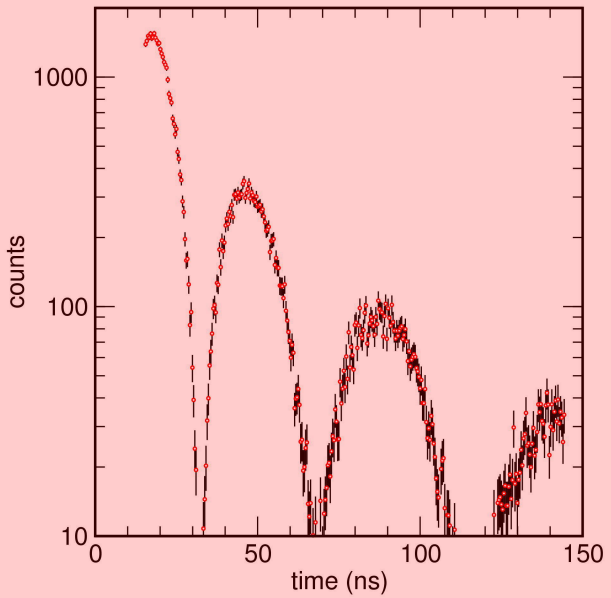
Fitting of SMS spectra:

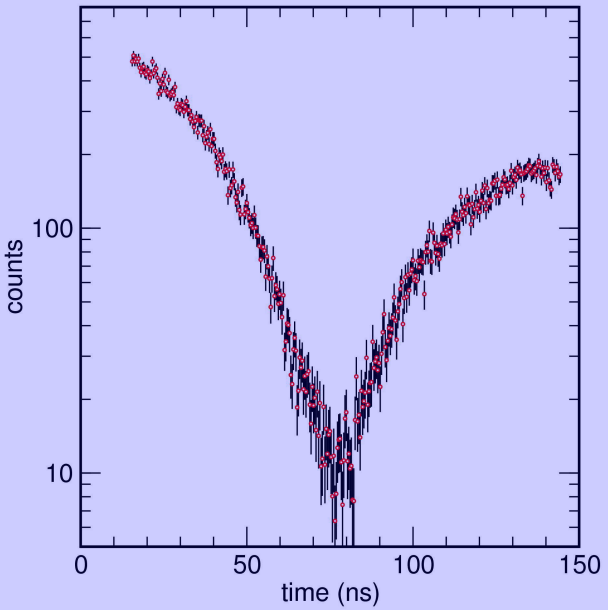
- strategy
  - identify relevant parameters
  - find start values using command `krmf`
  - optimize parameter values using `kctl`

- examples 1.2-4, 2.1-3, and 3.1-3
  - construct the input files in_kref, in_kmix, in_kfit, ex_in, in_kctl
  - focus on isomer shift, thickness, quadrupole splitting

SMS examples:

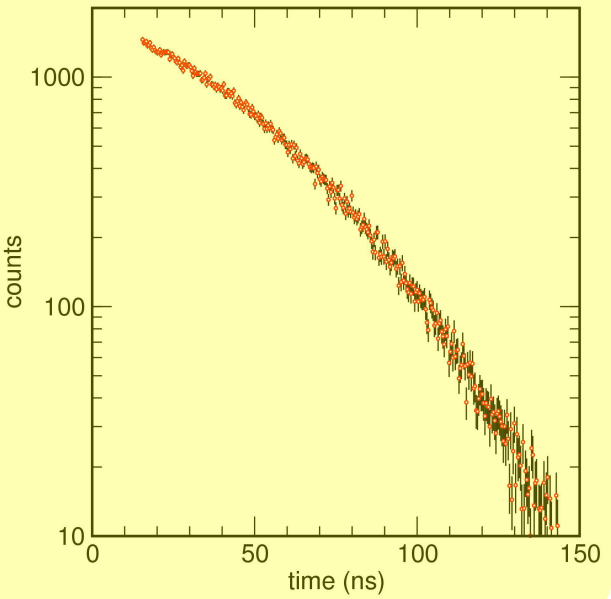
- example 1.2
  focus on thickness





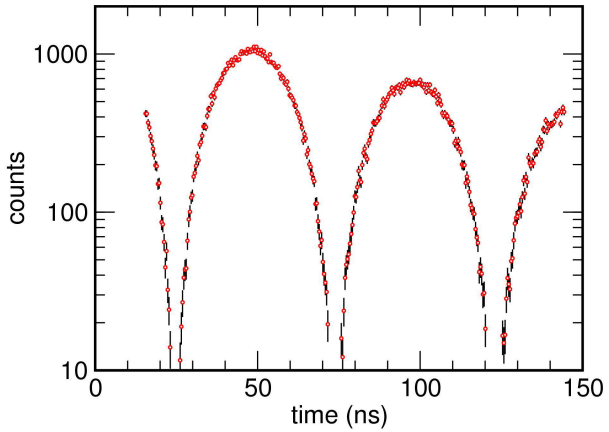
- example 1.3
  two sites; isomer shift;
  thickness 0.1µm

- example 1.4
  IS distribution;
  thickness 0.1µm

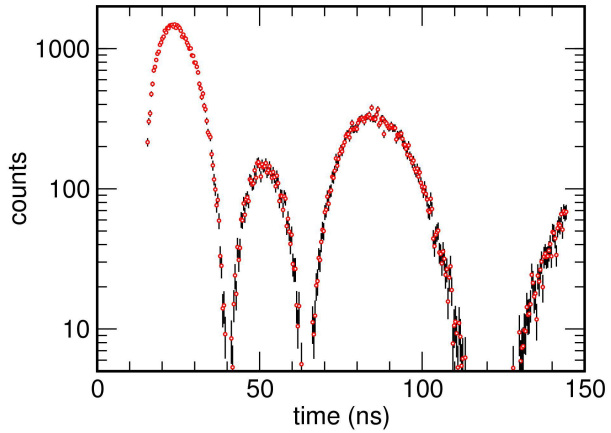


SMS examples, quadrupole splitting, isomer shift:

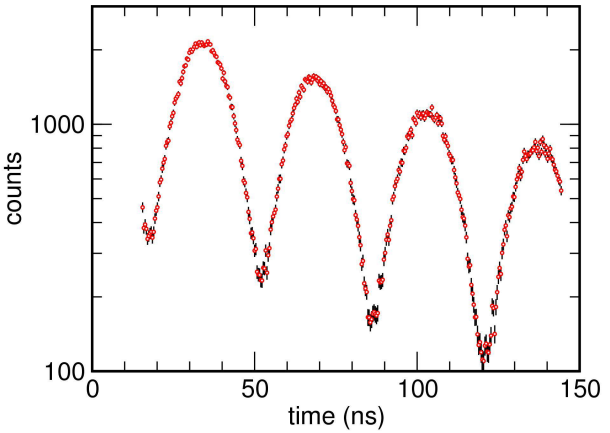
- example 2.1
  thickness 0.1µm



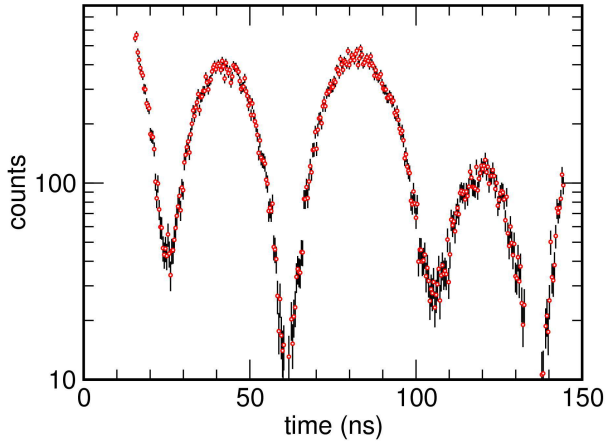
- example 2.2



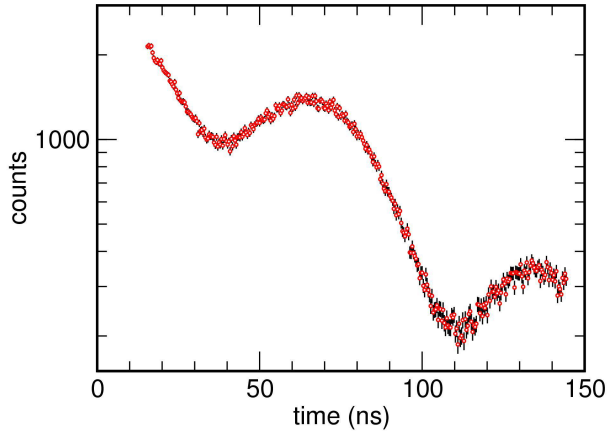
- example 2.3
  thickness 0.1µm; texture



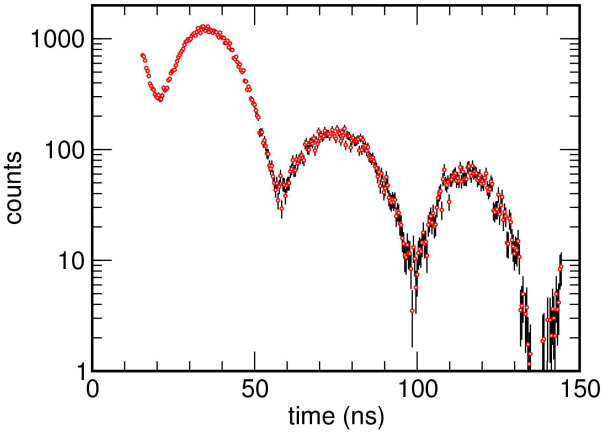
- example 3.1
  0.1µm; two sites



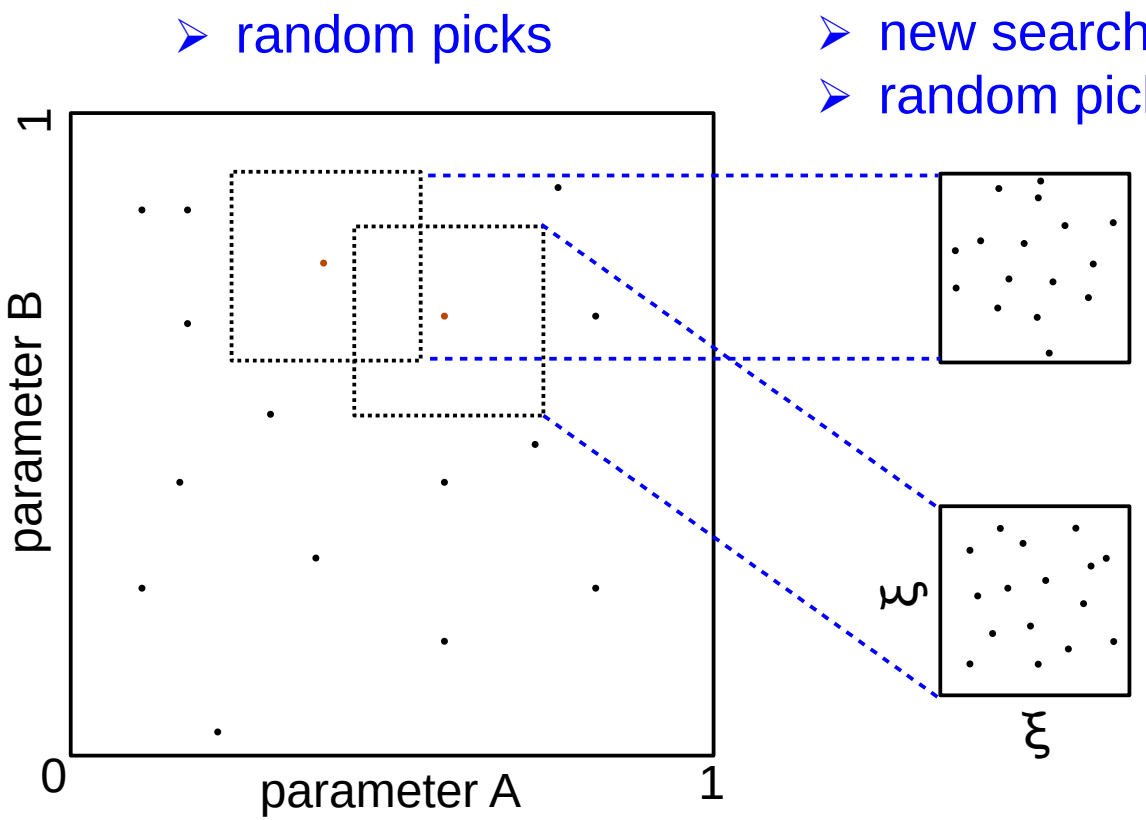
- example 3.2
  0.1µm; two sites



- example 3.3
  0.1µm; two sites; distr.

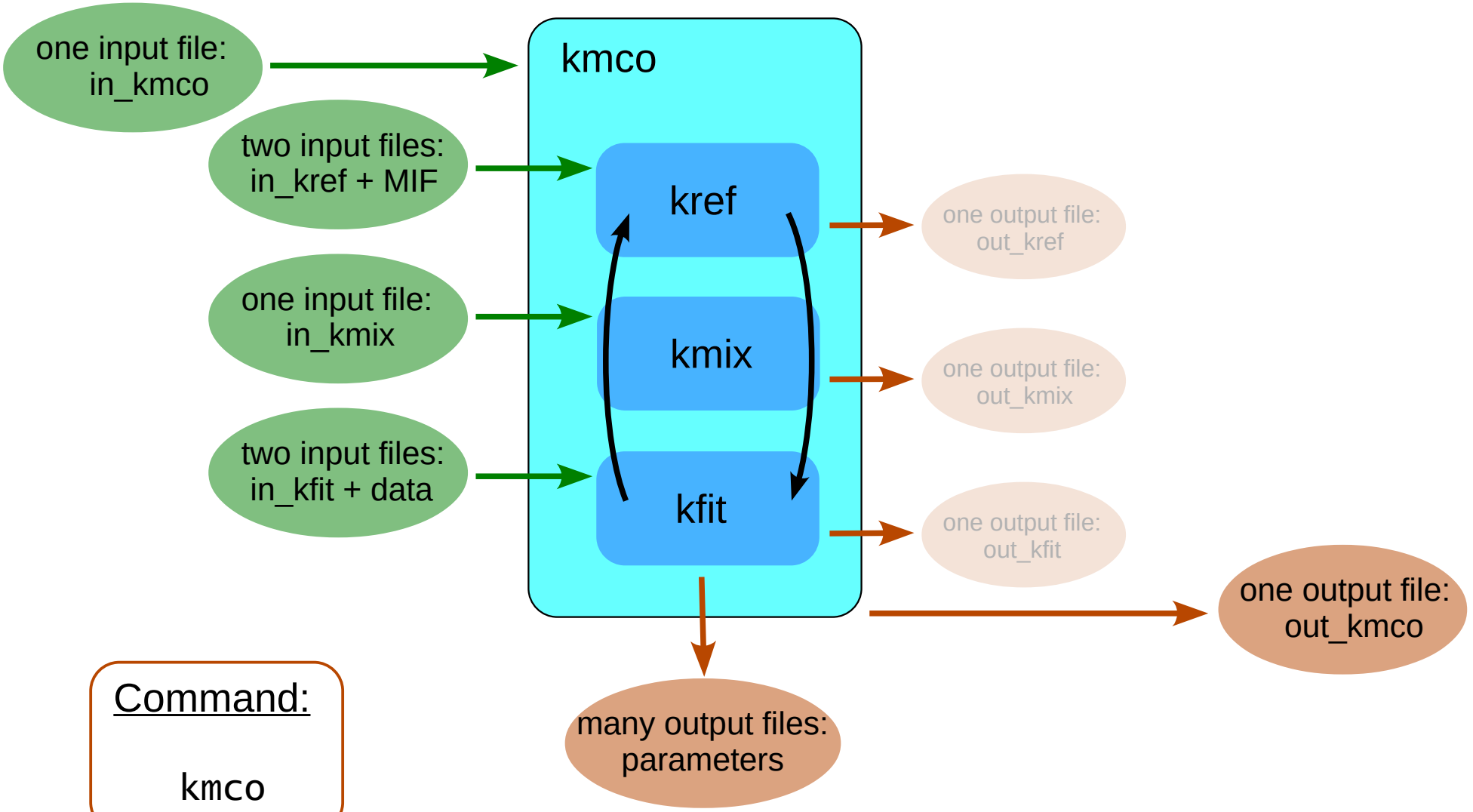


Randomized search:



☆ 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`

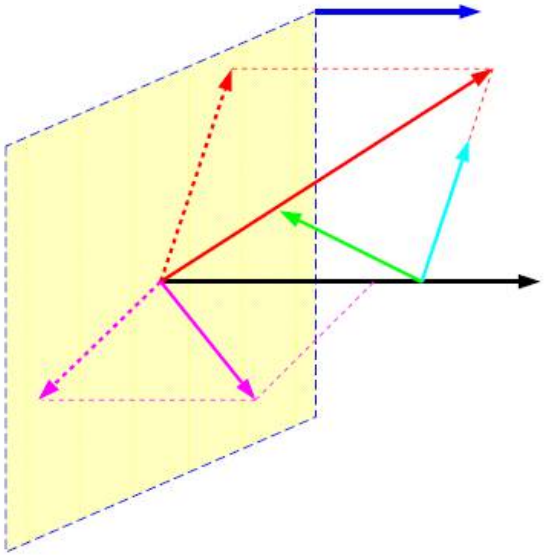
- redo examples that you found to be most difficult to fit
  - construct the input files in_kref, in_kmix, in_kfit, ex_in, in_kctl
  - focus on isomer shift, thickness, quadrupole splitting

End of Saturday's Class.

Tomorrow: Magnetic Fields

Polarization and field directions:

- polarization, defined by B_{ext}



(⟶) direction of incident radiation

(⟶) surface normal lines (8), (9), (10)

(⟶) direction of external magnetic field

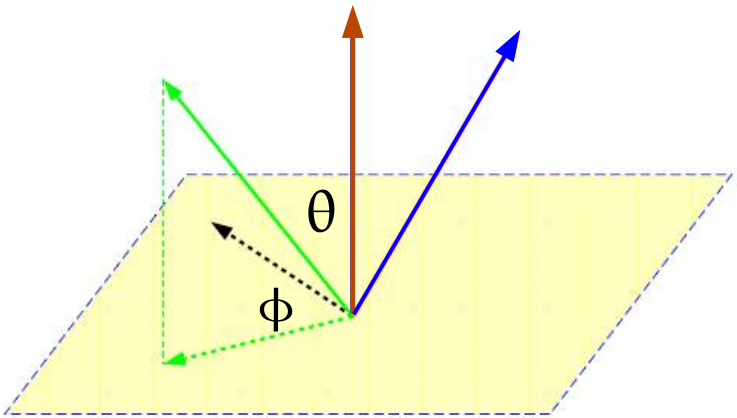
∠(⋮,⋮) = line (12) ∠(|,|) = line (13)

(⟶) = Sigma polarization

(⟶) = Pi polarization

(⟶) lattice base vector

- magnetic hyperfine field



(⟶) surface normal

(⟶) direction of external magnetic field

(⟶) cross product (⟶) X (⟶)

(⟶) direction of the magnetic hyperfine field

∠(|,|) = line (26.#.9) ∠(⋮,⋮) = line (26.#.10)

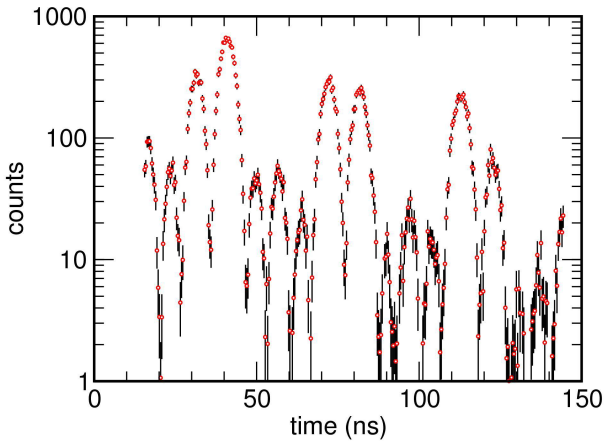
Magnetic SMS spectra:

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

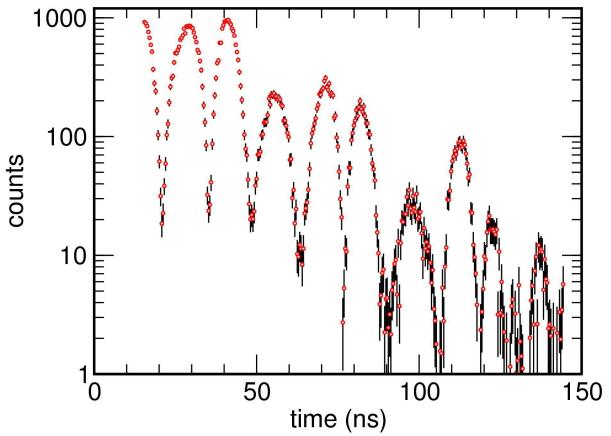
- examples 4.1-3 and 5.1-3
  - construct the input files in_kref, in_kmix, in_kfit, ex_in, in_kctl
  - focus on magnetic fields: magnitude, direction, and distribution

SMS examples, magnetic fields:

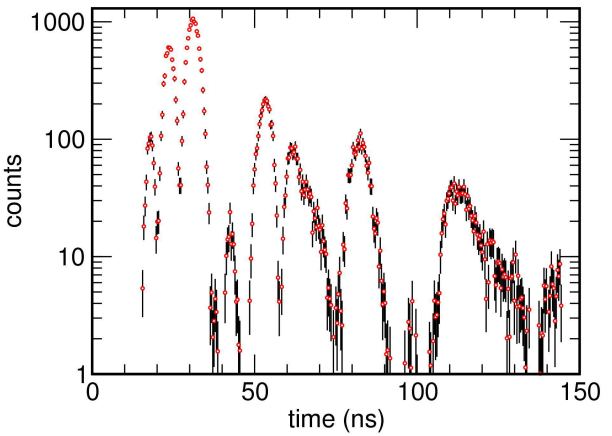
- example 4.1
  no texture



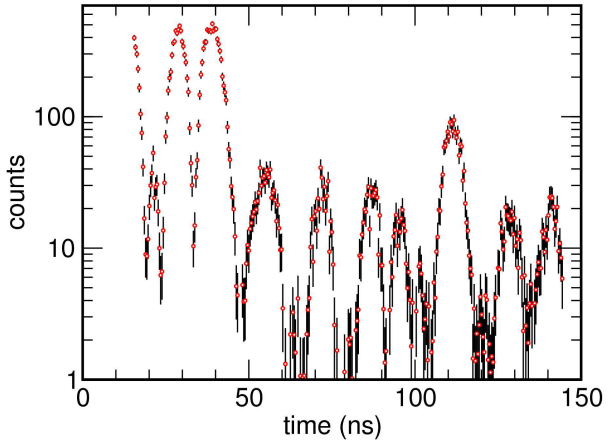
- example 4.2
  texture



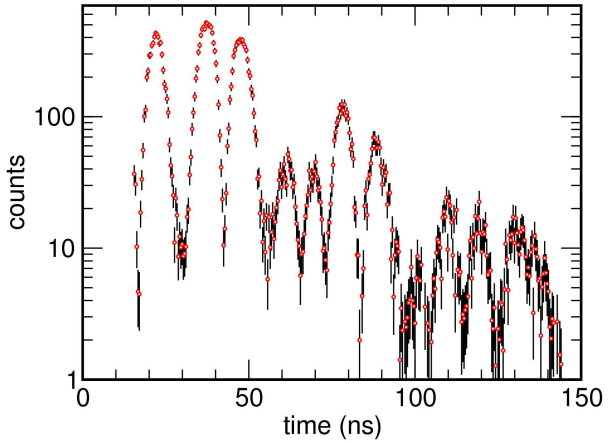
- example 4.3
  no texture; distribution



- example 5.1
  no texture



- example 5.2



- example 5.3