Analysis of Time-of-Flight Data via SAMMY

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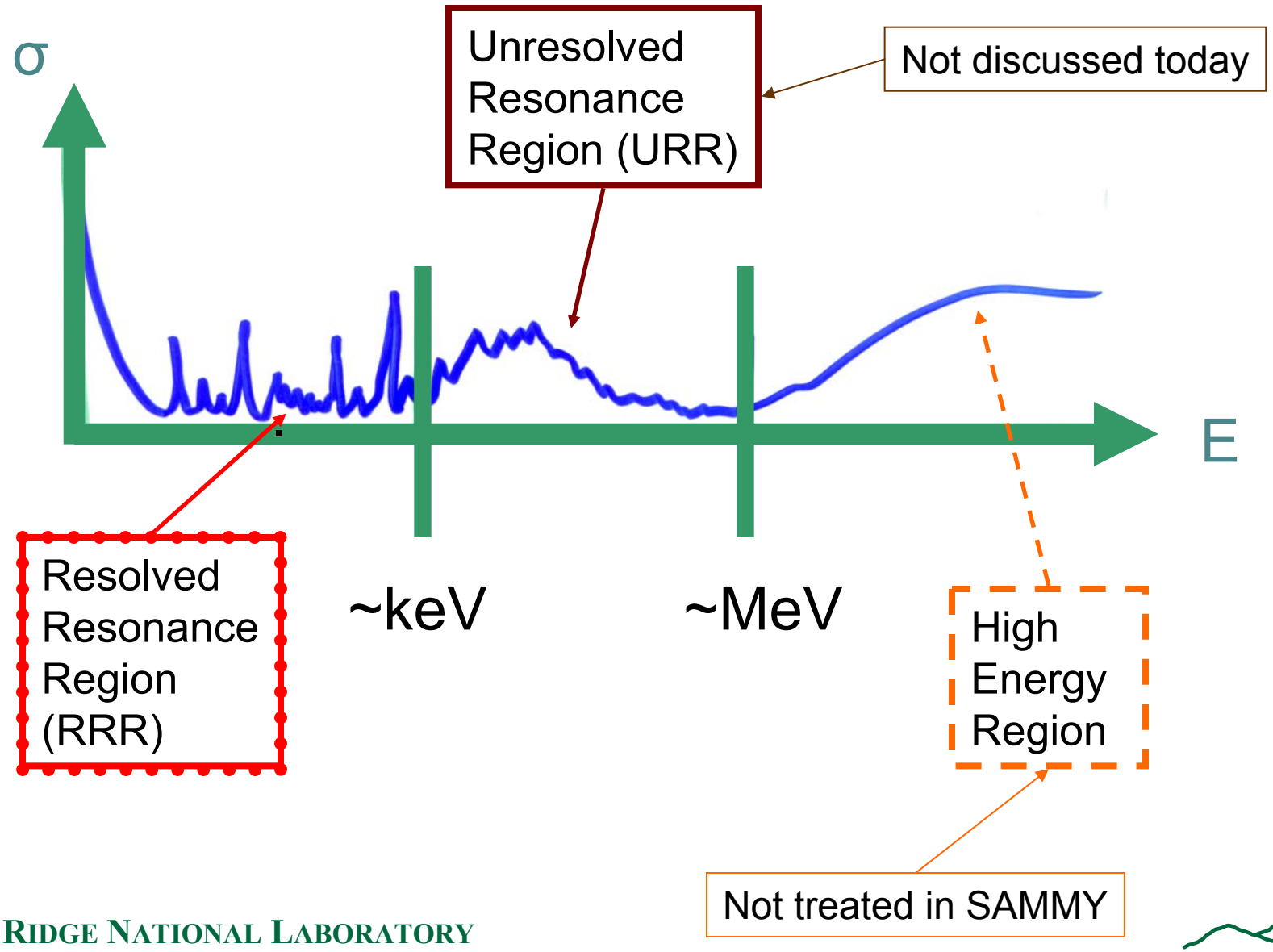
Outline of talk

- **Introduction**
- **Three requirements for analysis codes**
  1. **Theoretical cross sections**
  2. **Corrections for experimental conditions**
  3. **Fitting procedure**
- **Summary**

What is SAMMY?

- **SAMMY is a tool for analysis of time-of-flight cross section data in the resonance region**
  - **“tool” = “computer code”**


σ
Unresolved Resonance Region (URR)
Not discussed today
E
Resolved Resonance Region (RRR)
~keV
~MeV
High Energy Region
Not treated in SAMMY

Introduction, cont.

- ***Incident particles:***
  - **neutron, proton, alpha…**
- ***Target:*** **one type of nuclide, or many**
  - **Multiple isotopes**
  - **Chemical compounds**
  - **Contaminants**

Types of data

- **Total (transmission), elastic, capture, fission, inelastic, other reactions**

  energy-differential data

  - **Charged-particle entrance and/or exit channels**

- **Angular distributions**

  energy- and angle- differential data

- **Integral data (Westcott's g-factor, resonance integral, Watt spectrum average, K1, alpha)**

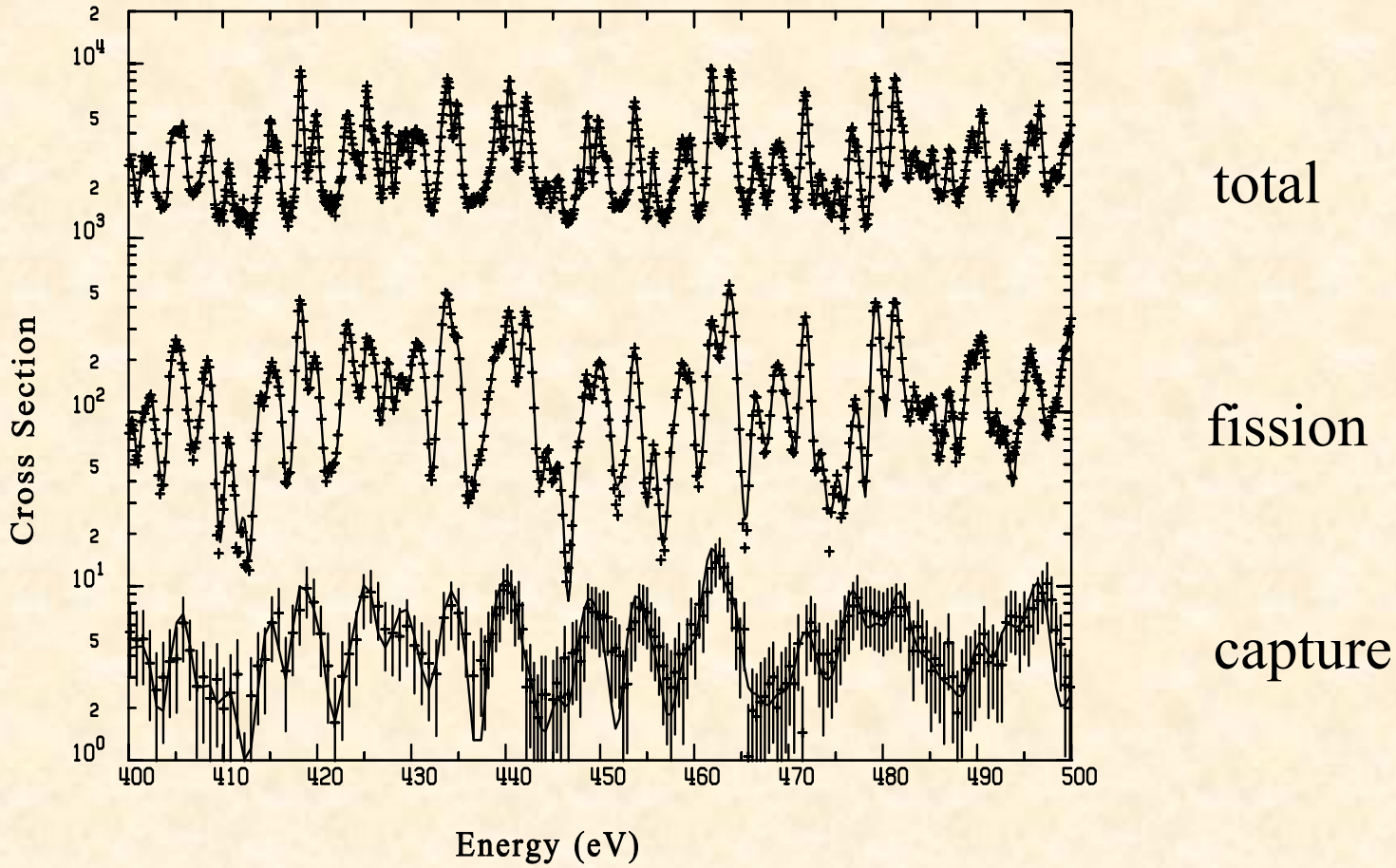
  energy- and angle-integrated data

Other observables (e.g. polarizability) may eventually be added.

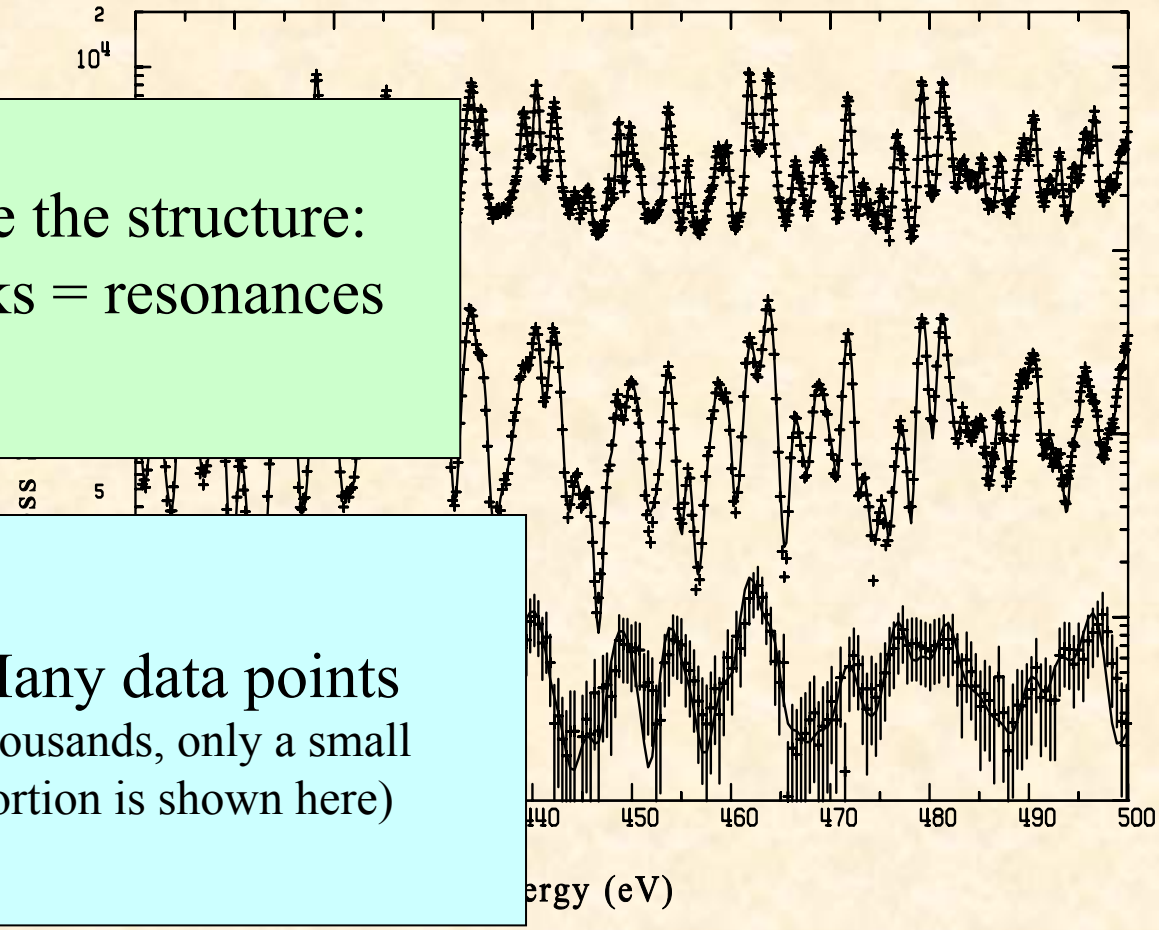
What do the data look like?

- **Numbers!**
  - **Energy**
  - **Cross section**
  - **Uncertainty (covariance)**

- **Next slide shows one example, three data types…**



^{235}U experimental and calculated total cross section, fission cross section, and capture cross section in the energy range from 400 to 500 eV. Harvey et al. total cross section (multiplied by 100), Weston fission (multiplied by 10), and deSaussure capture cross sections are displayed.



Note the structure:
peaks = resonances

Many data points
(thousands, only a small portion is shown here)

total

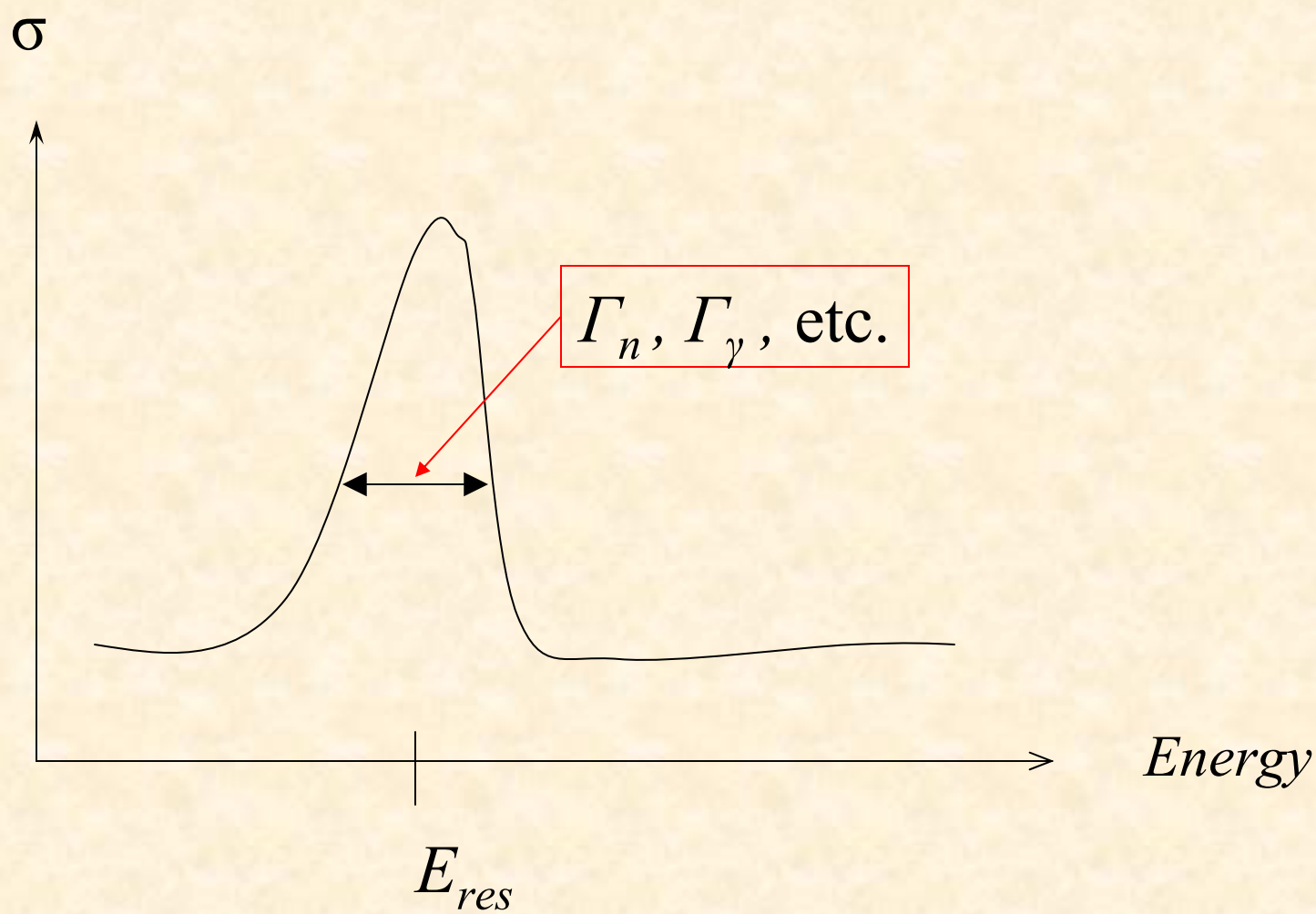
fission

capture

^{235}U experimental and calculated total cross section, fission cross section, and capture cross section in the energy range from 400 to 500 eV. Harvey et al. total cross section (multiplied by 100), Weston fission (multiplied by 10), and deSaussure capture cross sections are displayed.

Objective of SAMMY

- **Describe the data in terms of physical parameters for each resonance**
  - **Energy E_{res}**
  - **Neutron width Γ_n**
  - **Capture width Γ_γ**
  - **Quantum numbers $l\ s\ J\ \pi$**
- **Find values and uncertainties (and correlations) for these parameters**
- **Report results to Evaluated Nuclear Data Files**


σ
Γ_n, Γ_γ, etc.
Energy
E_{res}

Why parameterize the cross sections? Why not just use the measured data?

- **Too much information, too little understanding**
  - **cross section vs. energy ➔ ~100,000's of numbers**
  - **angular distributions have even more numbers**
  - **human minds seldom make sense of this many numbers!**

- **Not enough information ➔ extrapolations are needed for practical applications**
  - **other energies (into the unresolved resonance region)**
  - **other experimental conditions:**
    - **temperature (Doppler broadening)**
    - **geometry**
      - **self-shielding calculations, multiple-scattering effects, etc.**
  - **other nuclides (? This is dangerous in resonance region!)**

Purpose of SAMMY

- **Provide the parameterization**

  by analyzing time-of-flight cross-section data

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Requirements for Analysis

Analysis of neutron cross-section data in resolved-resonance region has three requirements:

1. **Formalism for calculation of cross sections**
2. **Mathematical description of experimental effects**
3. **Fitting procedure, including treatment of covariances**

Numbers 1 & 3 are "relatively easy"

(even though we don't always do them correctly)

Number 2 is impossible!

(all we can do is make better and better approximations)

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1. Formalism for Calculating Cross Sections

- **Reich-Moore Approximation to Multi-Level Multi-Channel R-Matrix Theory**
  - **For a single resonance, with *a* = entrance channel and *b* = exit channel, the formula is**

$$\sigma_{a \to b} = \frac{\pi}{k^2} g \frac{\Gamma_a \Gamma_b}{\left(E_{res} - E\right)^2 + \left(\Gamma / 2\right)^2}$$

where Γ is the sum of all the widths.

Formalism , cont.

Reich-Moore Approximation to Multi-Level Multi-Channel R-Matrix Theory

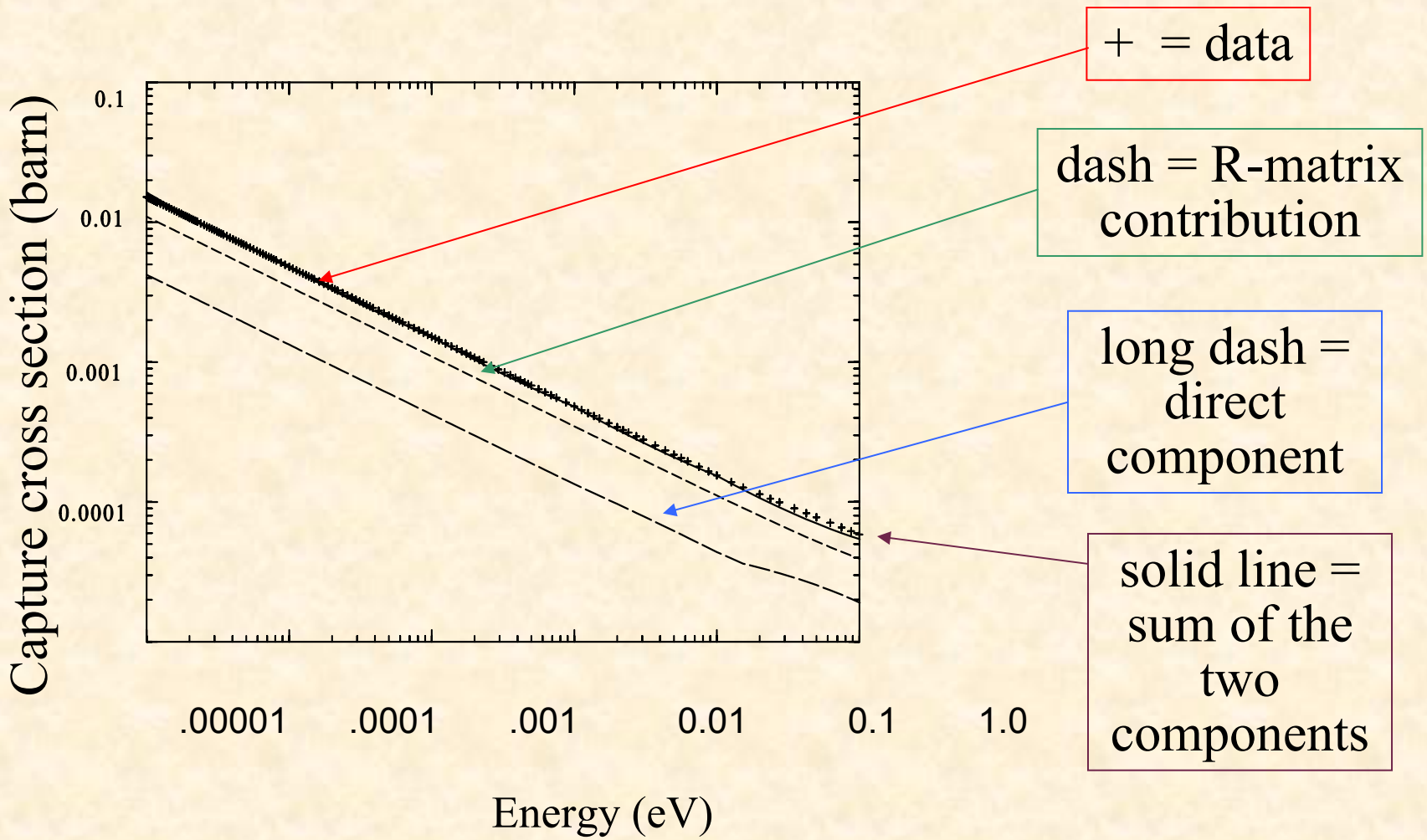
F. H. Fröhner, "Evaluation and Analysis of Nuclear Resonance Data," JEFF Report 18 (2000), page 60:

"Experience has shown that with this [Reich Moore] approximation all resonance cross section data can be described in detail, in the windows as well as in the peaks, even the weirdest multilevel interference patterns … It works equally well for light, medium-mass and heavy nuclei, fissile and nonfissile."

When does Reich-Moore *not* work ?

- **For direct effects**
  (R-matrix is a description of *compound* nucleus effects.)
  - **Must be added explicitly**
  - **New options are now available in SAMMY for fitting the magnitude of direct capture component**
  - **Example on next page for ^{19}F**
    - **Model calculations by Goran Arbanas, ORNL**
    - **Analysis by Luiz Leal, ORNL**
      - **Multiplier initially at 1.0, fitted to 0.547**

^{19}F, continued



When does Reich-Moore *not* work ? (continued)

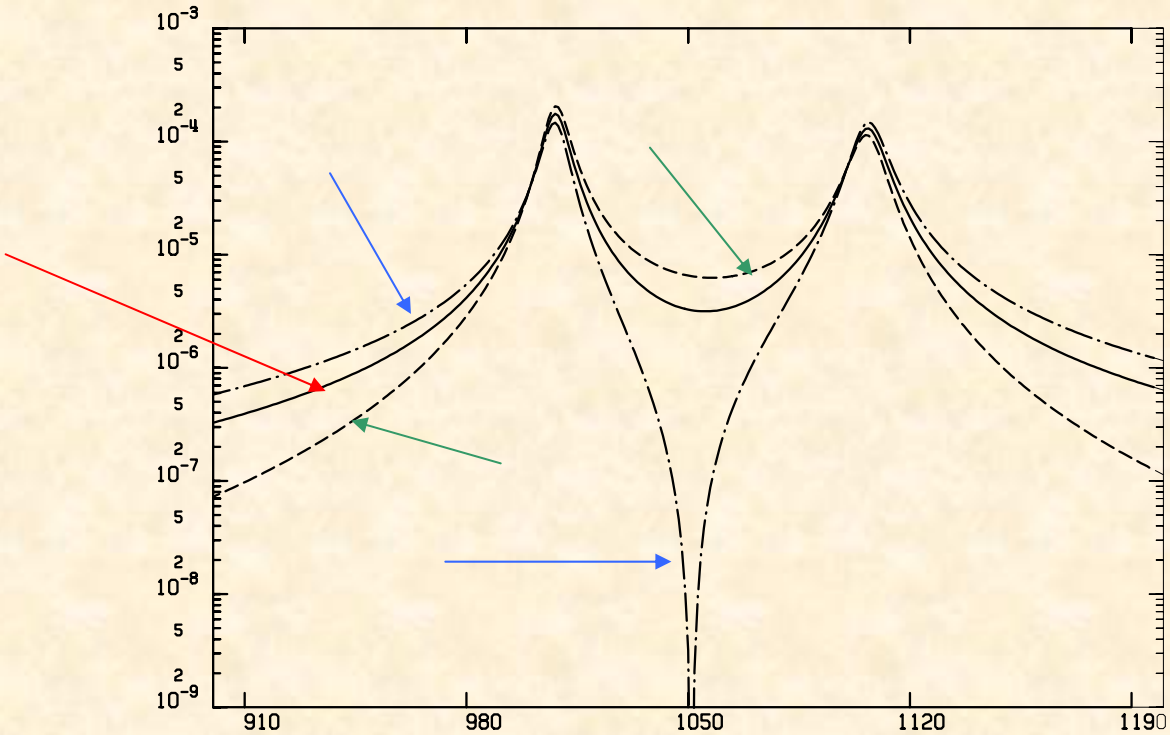
- **When trying to describe interference effects in reactions like**
  - **$^{12}C(\alpha,\gamma)$**
  - **$^{15}N(p,\gamma)$**
  - **$^{21}Ne(p,\gamma)$**
  - **$^{22}Ne(n,\gamma)$**

when there is level-level interference in the capture channel

because capture is treated "on average" in Reich-Moore approximation

  - **re Michael Heil, Karlsruhe**

Artificial example is shown on next slide



Solid line = Reich Moore

Dot-dash = full R-matrix # 1

Dash = full R-matrix # 2

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2. Description of Experimental Conditions

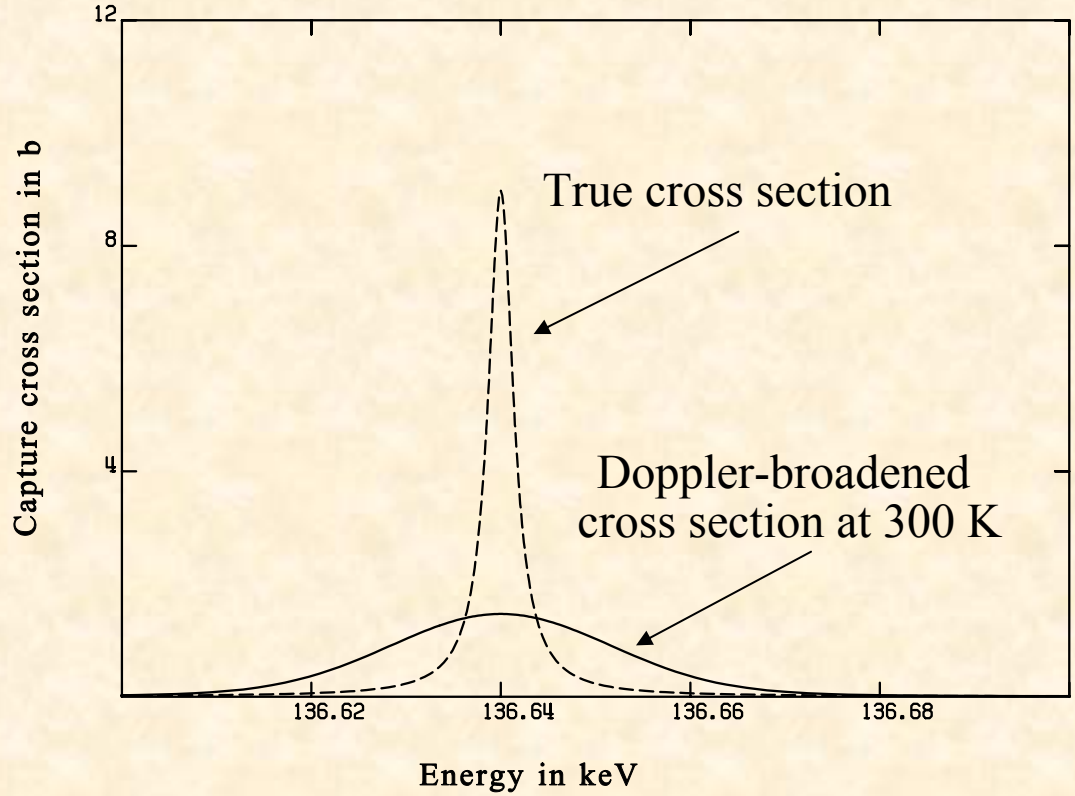
Code must simulate experimental conditions which cause measured cross section to be different from true cross section

Doppler Broadening

finite temperature

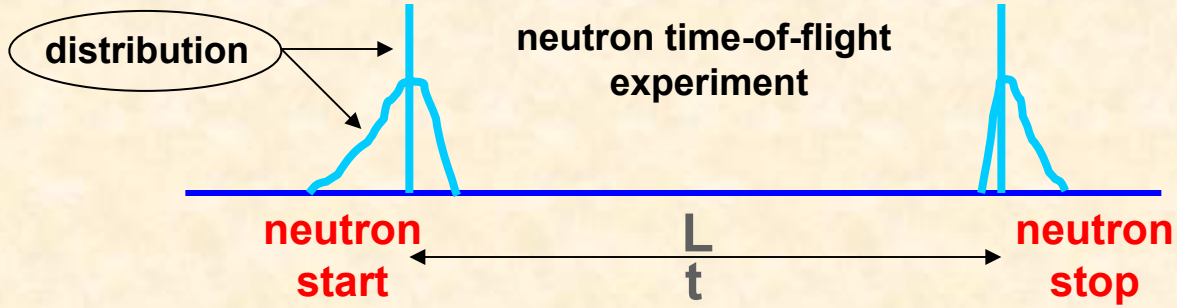
- **FGM: Free gas model**
- ~~**HEGA: High-Energy Gaussian Approx to FGM**~~

  ~~**(Please do NOT use!)**~~
- **CLM: Crystal lattice model has been implemented**



Resolution broadening

What is resolution?



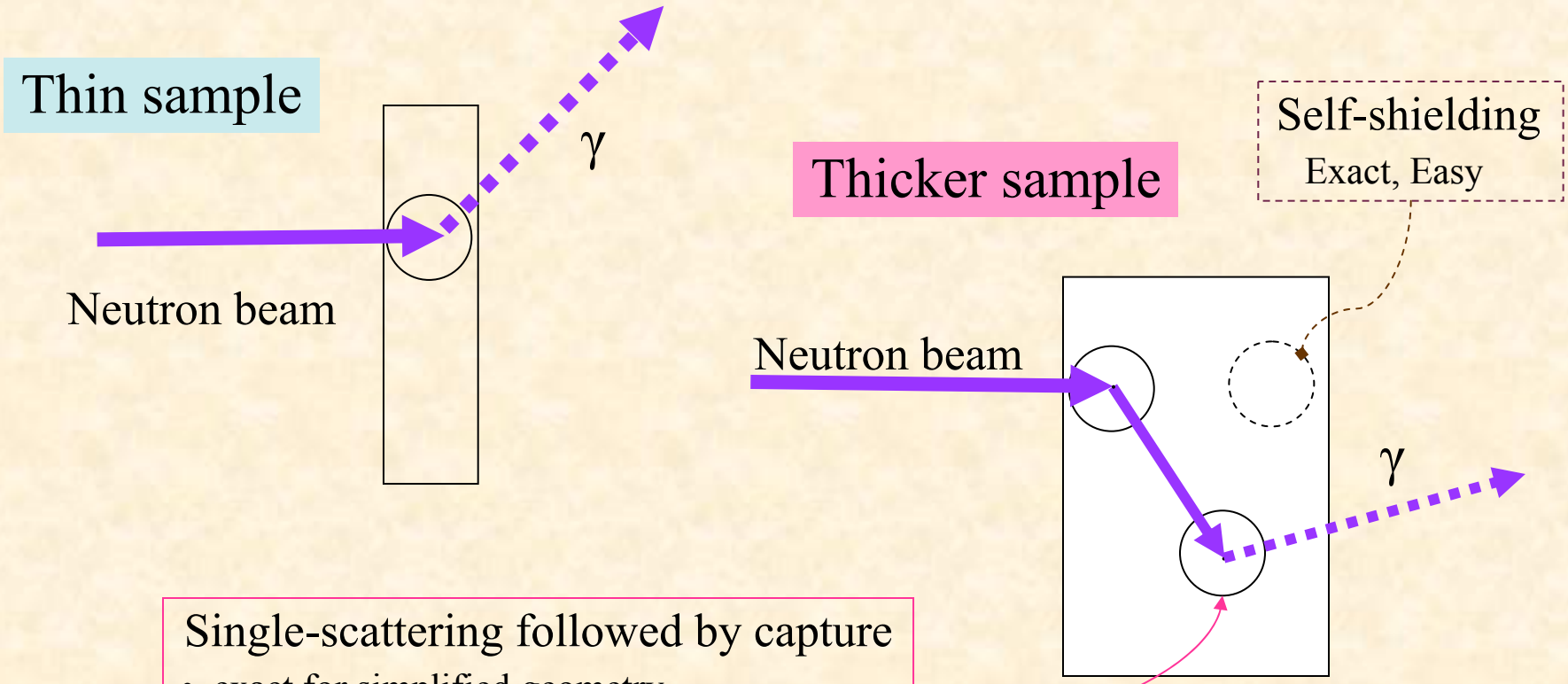
Picture stolen from Frank Gunsing, Saclay

Resolution Broadening in SAMMY

(Unlike Doppler broadening, resolution broadening is different for each experiment.)

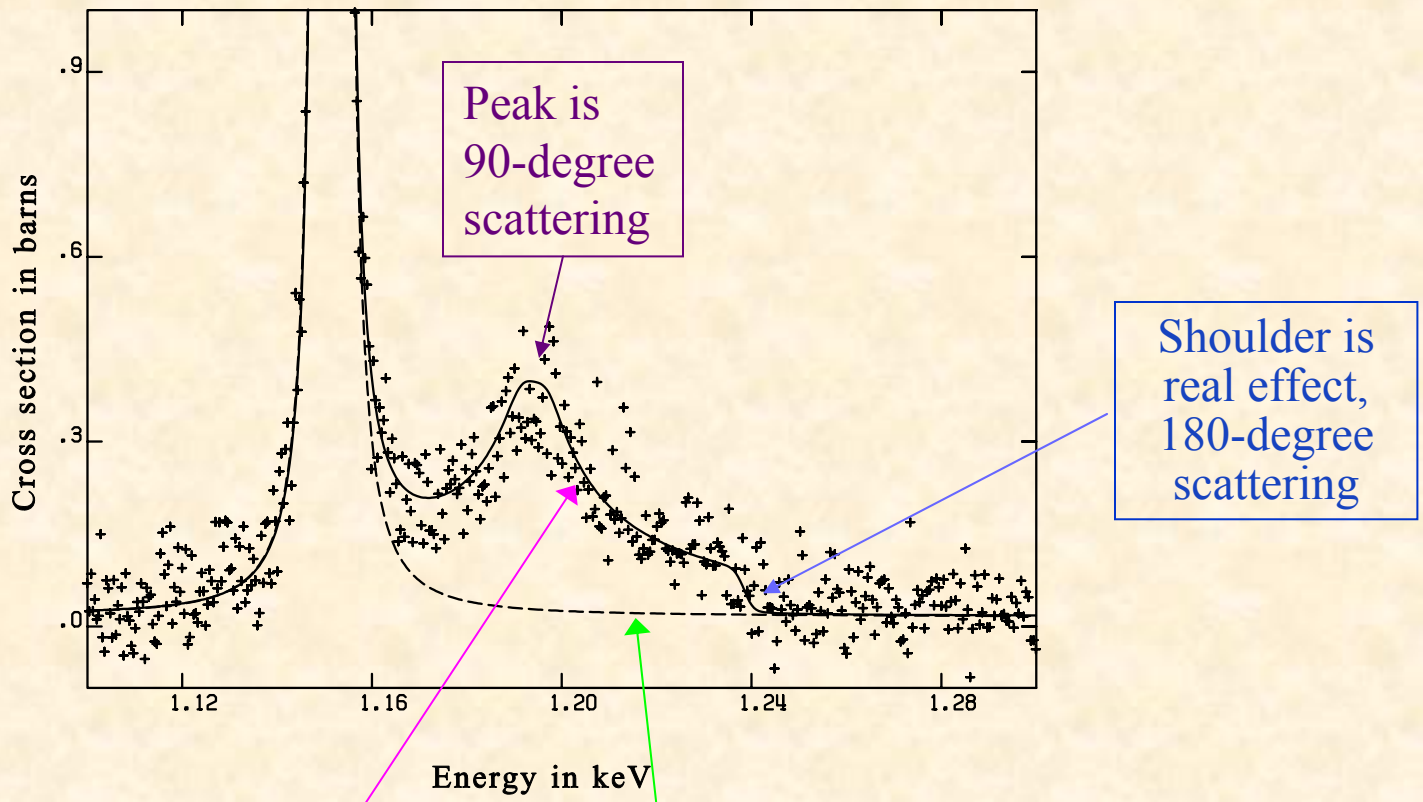
- **Quick-&-easy version (Gaussian + exponential tail) (RSL)**
- **Oak Ridge resolution function (ORR)**
- **RPI resolution function (RPI)**
  - **[New extension is useful for Geel or n_TOF data as well]**
- **Energy-average from E to E - Δ (DEX)**
- **Numerical User-Defined Resolution function (UDR)**
  - **[implemented but not fully functional]**
- **Combinations RSL + DEX + one of {ORR, RPI, UDR}**

Multiple Scattering Corrections for fission and capture experiments



Single-scattering followed by capture

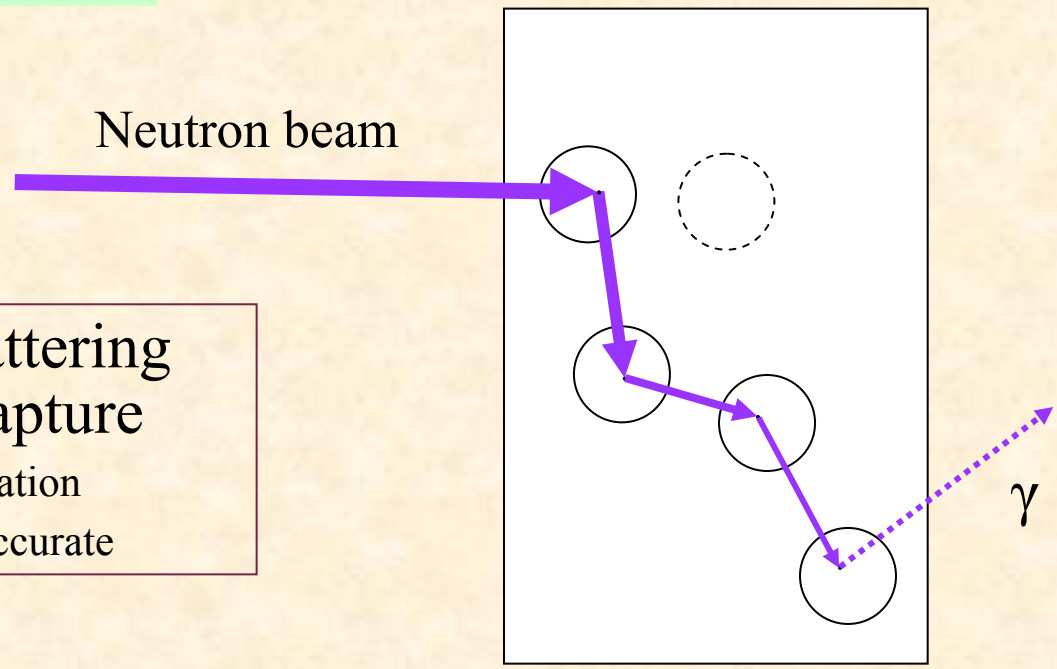
- exact for simplified geometry
- complicated mathematics
- complicated coding
- simplifies if target is infinite slab



The 1.15-keV ^{56}Fe resonance in natural iron capture data of R. Spencer et al. Dashed curve is SAMMY calculation without self-shielding or single-scattering correction; solid curve includes those corrections.

Multiple Scattering Corrections for fission and capture experiments, cont.

Thicker sample yet, multiple scattering



double-plus scattering followed by capture

- gross approximation
- not particularly accurate

Normalization and Background Corrections

- **Constant normalization**
- **Many varieties of energy-dependent background**

Multiple Nuclides

Parameters must be specified for each nuclide

- **R-matrix parameters**
- **Identifiers such as mass, spin, charge**
- **Abundance**

- **SAMMY treats nuclides appropriately**
  - **Doppler broadening now done properly for each nuclide (mass-dependent)**
  - **Multiple-scattering corrections etc. calculated for each nuclide**

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3. Fitting Procedure (Bayes' method)

(or generalized least-squares)

$$P' = P + M' Y \qquad M' = (M^{-1} + W)^{-1}$$

$$Y = G^t V^{-1} (D - T) \qquad W = G^t V^{-1} G$$

Notation: (primes indicate updated values)

P = parameters
M = covariance matrix for parameters
D = experimental data
T = theoretical calculation
G = partial derivatives (sensitivity matrix)
V = covariance matrix for experimental data

Compare to least squares –

Bayes' method	Least Squares
$P' = P + M' Y$ $\quad M' = (M^{-1} + W)^{-1}$ $Y = G^t V^{-1} (D - T)$ $\quad W = G^t V^{-1} G$	$M' = W^{-1}$
M = initial covariance matrix for parameters	M = infinite "no prior knowledge"
Remembers earlier results	Forgets
Use results of one analysis as input to another	Cannot
Results from sequential analyses are "identical" to those obtained from simultaneous analysis (subject to linearity restrictions)	Not
OK to vary irrelevant parameters; values and uncertainties will change only slightly	Wastes time trying to find "good values" for irrelevant parameters

Data Covariance Matrix = *V*

is the sum of two terms

- **Statistical** diagonal
  - **come from the measurement process**
  - **generally Poisson statistics**

- **Systematic** off-diagonal but separable

  (Fröhner calls these "common errors")
  - **occur because raw data have been modified (by background subtraction, normalization, etc.)**

Data Covariance Matrix, continued

Statistical part; diagonal

Complete data covariance matrix is

$$V = v + g\,m\,g^{t}$$

Systematic, off-diagonal

where

- ***V* is the data covariance**
- ***v* represents the statistical uncertainties**
- ***g* is the sensitivity matrix (partial derivative of data with respect to data-reduction parameters)**
- ***m* is the covariance matrix for the data-reduction parameters**

(What are these data-reduction parameters?)

- **used for describing experimental conditions**
  - **normalization, background**
  - **burst width**
  - **isotopic abundance**
  - **etc.**
- **can be used in two ways**
  - **used to generate data covariance matrix**
  - **included as varied parameters in fitting procedure**
    - **mathematically equivalent to using data-covariance matrix**
    - **numerically more stable**
    - **bonus: provides better estimate of value of parameter**

Inverting the data covariance matrix *V*

- **Usual method of treating *V* is to calculate it explicitly using**

$$V = v + g\, m\, g^{t}$$

and then explicitly invert it to give V^{-1}

- **A better method is to symbolically invert it using the pieces**

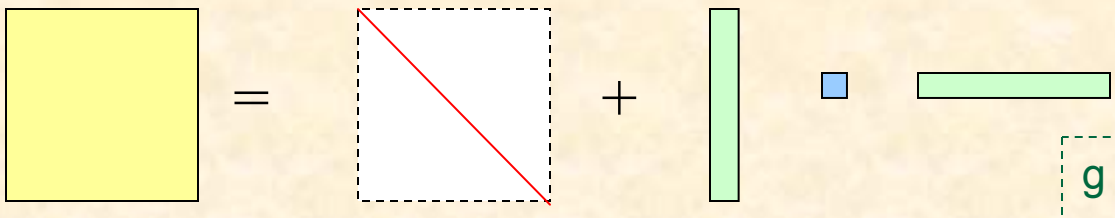
Implicit data covariance (IDC)

Data Covariance Matrix, symbolically

Statistical part

Systematic part

$$V = v + g\ m\ g^t$$



g = sensitivity for data-reduction parameters
m = cov matrix for d-r par

where

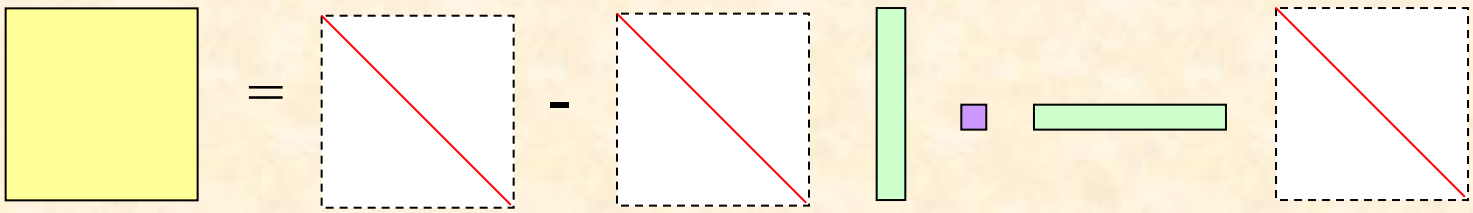
- **size of box may be considered to be logarithmic**
  - **large ~ thousands (or 10 K or 100 K)**
  - **small ~ very few (5? 10?)**
- **dashed box with diagonal line indicates diagonal matrix**
- **solid box indicates non-diagonal matrix**

Inverse of Data Covariance Matrix, symbolically

$$V^{-1} = (v + g\ m\ g^t)^{-1}$$

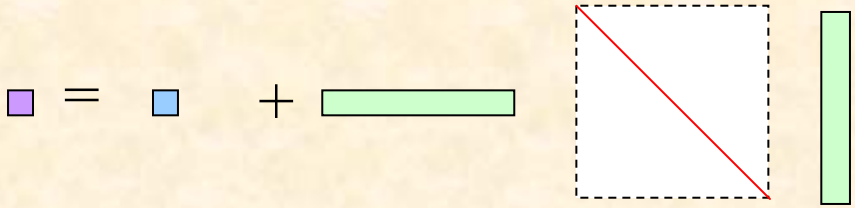
$$= v^{-1} - v^{-1} g\,(m^{-1} + g^t v^{-1} g)^{-1} g^t v^{-1}$$

$$= v^{-1} - v^{-1} g\ Z^{-1}\ g^t v^{-1}$$



where

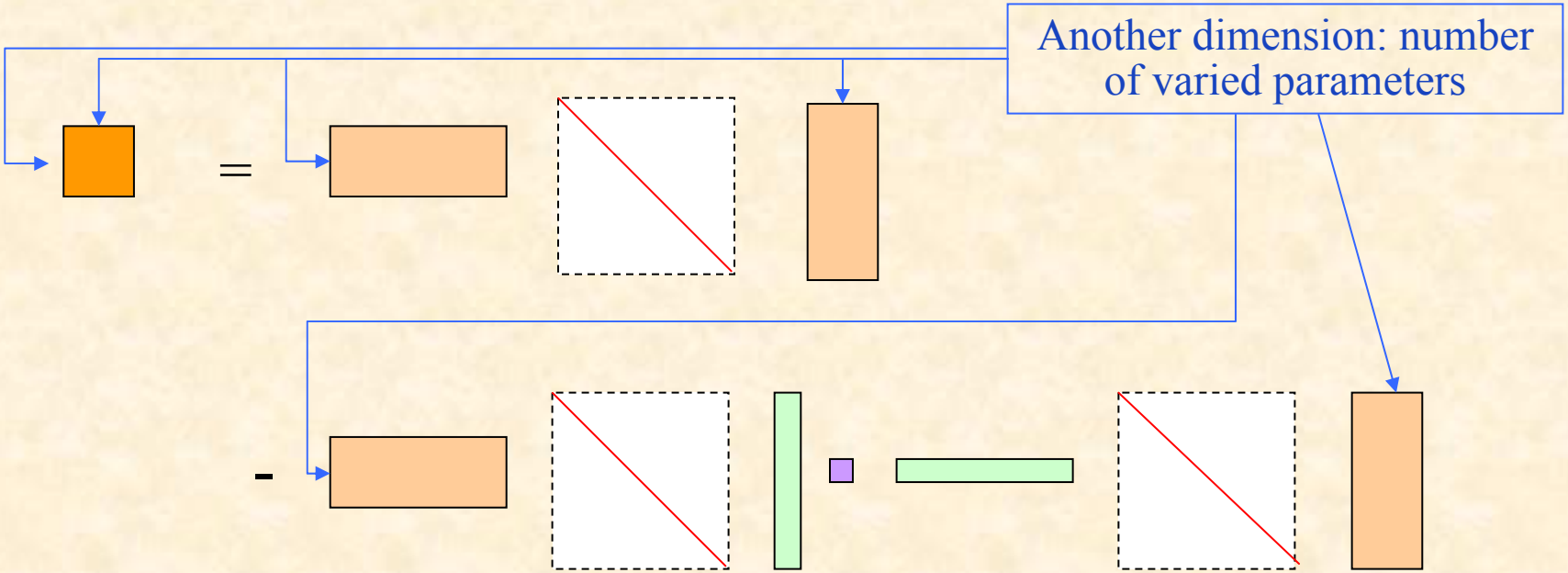
$$Z = m^{-1} + g^t v^{-1}\ g$$



Quantities needed in Bayes' equations: W

$$W = G^t V^{-1} G$$

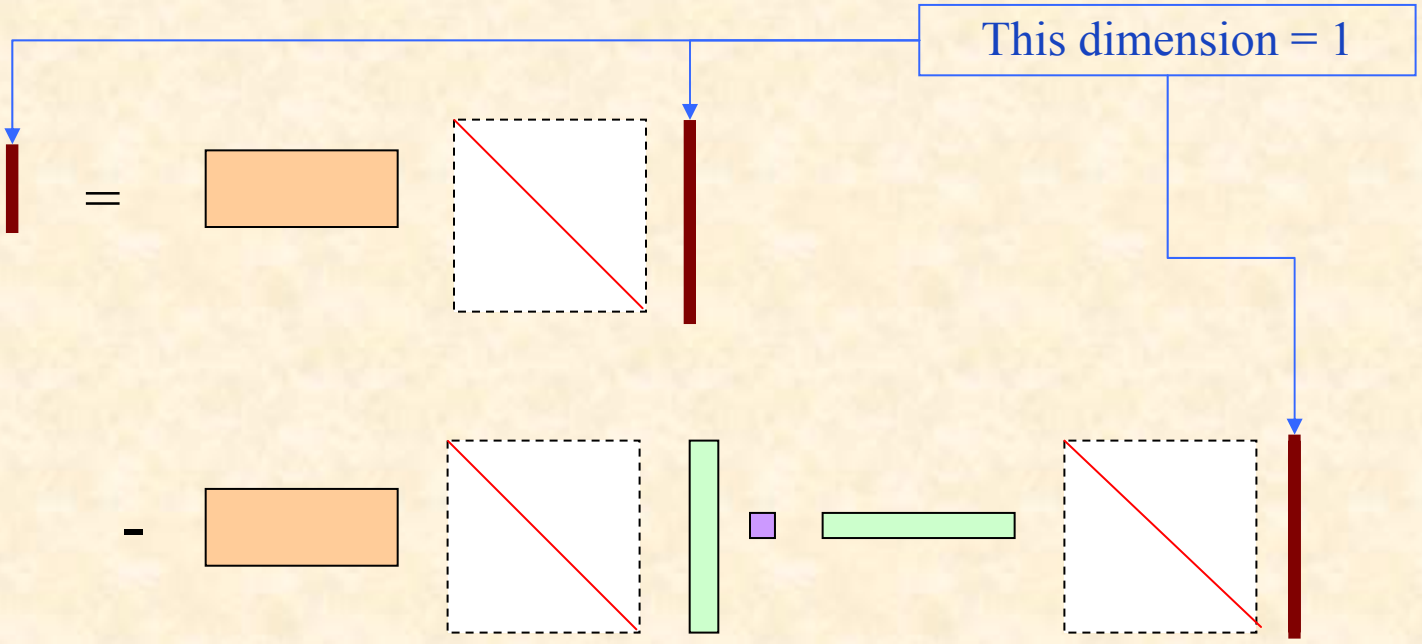
$$= G^t v^{-1} G - G^t v^{-1} g Z^{-1} g^t v^{-1} G$$



Quantities needed in Bayes' equations: Y

$$Y = G^t V^{-1} (D - T)$$

$$= G^t v^{-1} (D - T) - G^t v^{-1} g Z^{-1} g^t v^{-1} (D - T)$$



Why bother with all these arrays?

Matrices in *W* and *Y* are easier to invert than *V* –

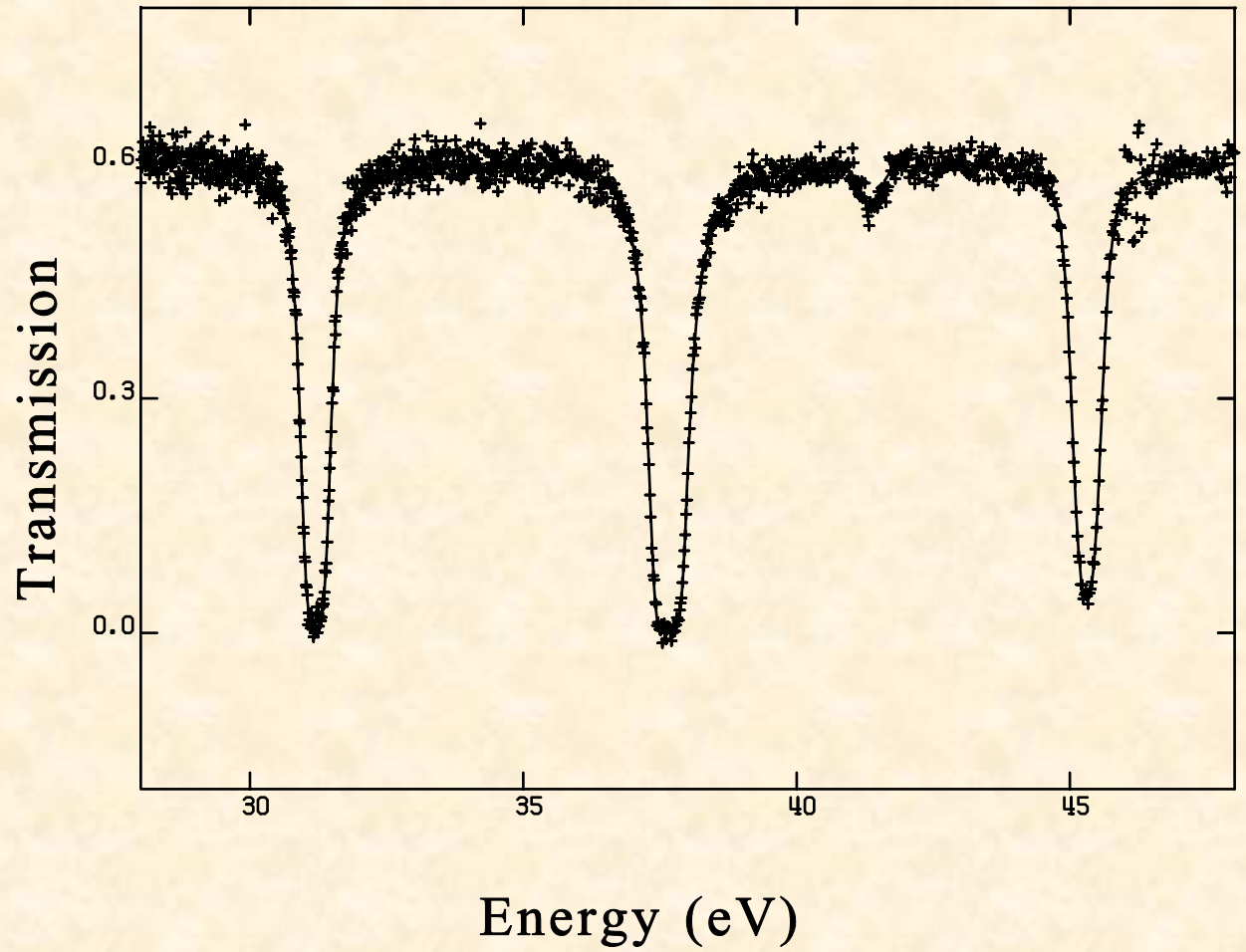
- ***v* is large but diagonal**
  - **(size ~ thousands of data points)**
- ***m* is small and often diagonal**
  - **(size ~ tens of data-reduction parameters)**
- ***Z* is off-diagonal but small**
  - **(size ~ tens)**

– which leads to savings in

- **computation time (never calculate *V* or V^{-1})**
- **computer memory (never store *V* or V^{-1})**
- **numerical accuracy and stability (fewer round-off problems)**

Example from SAMMY Test Case tr140: ^{129}I transmission data

Geel data provided by Gilles Noguere, Cadarache



Example, continued

1245 experimental data points;
[full data set has 32660 data points]
9 data-reduction parameters;
655 resonances; 9 varied parameters in this example

	Description of data covariance treatment for this run	Cpu time for Bayes solver (sec)	Total cpu time (sec)	Array size
a	only statistical errors	0.03	14	254 K
b	statistical plus systematic, only on diagonal	0.03	14	254 K
c	explicit data cov matrix	16.46 = x 500	59	1800 K = x 6
d	IDC matrix	0.06 = x 2	14	267 K = x 1.1

Note: c & d give essentially the same results provided c is done carefully

In SAMMY, **implicit data covariance (IDC) matrices** can be used for

- **normalization and background correction factors**
- **user-supplied implicit data covariance**
  - **external code can be used to generate pieces (*g* and *m*)**
- **propagated-uncertainty parameters (PUPs)** new

To simultaneously analyze several data sets – rewrite Bayes' Equations

$P' = P + M' Y$ where $Y = \Sigma_i Y_i$

with $Y_i = G^t V^{-1} (D - T)$ for data set i

$M' = (M^{-1} + W)^{-1}$ where $W = \Sigma_i W_i$

with $W_i = (G^t V^{-1} G)$ for data set i

- **Treat individual data sets separately, calculating Y_i and W_i**
- **Add to give Y and W**
- **Solve Bayes' equations *once* to fit all data sets**

Simultaneous analyses, continued

- **Currently in SAMMY**
  - **Can more-or-less do simultaneous analyses**
    - **Awkward – requires several different SAMMY runs**
    - **Cannot iterate to take care of non-linearities**
  - **Is used primarily for retroactive calculation of approximate resonance parameter covariance matrix**

for ENDF file 32

- **Eventually**
  - **Restructured SAMMY will permit truly simultaneous analyses of any number of experimental data sets**
    - **This requires major changes both internally in the code and in the input**

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Summary

Three requirements for analysis of time-of-flight cross section data:

1. **Formalism for calculation of cross sections**
2. **Mathematical description of experimental effects**
3. **Fitting procedure, including treatment of covariances**

Want to learn more?

- **SAMMY Workshops**
  - **Format**
    - **Detailed lectures (~15 hours)**
      - **Covering all aspects of analysis via SAMMY**
    - **Tutorial exercises on the computer**
      - **Designed to teach step-by-step how to run the code**
  - **Where / when?**
    - **North Carolina State University, 2005**
    - **ICTP in Trieste, Italy, February or March 2006**

Ask for the workshop announcement

The End