Monte Carlo Rate Propagation for Experimentalists

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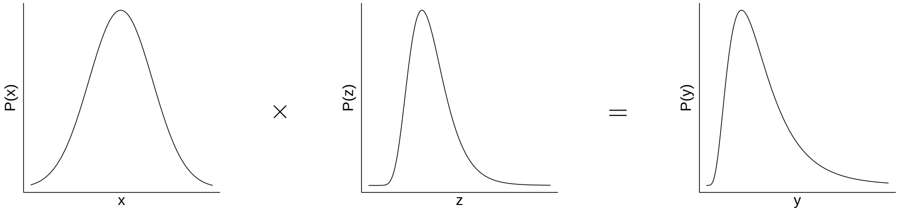
Monte Carlo Error Propagation

Reaction Rate per Particle Pair

$$\langle \sigma v \rangle = \sqrt{\frac{8}{\pi \mu}} \frac{1}{(kT)^{3/2}} \int_0^\infty E\sigma(E) e^{-E/kT} dE$$

$x \cdot z = y$



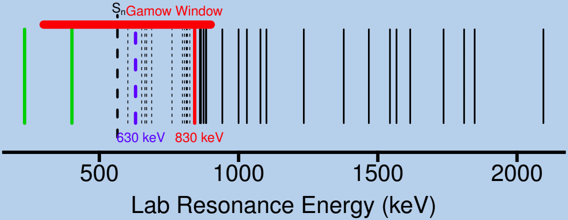
- Draw a random number from each distribution
- Perform calculation
- Repeat (1) and (2) many times
- Analyse final y-distribution

$$x = 0.5,\ z = 3.2$$
$$y = 1.6$$
$$y = 1.5, 2.3, 1.2, 1.4, 1.2, 1.8, 1.6, 1.5, 2.0$$

Median $y = 1.6$

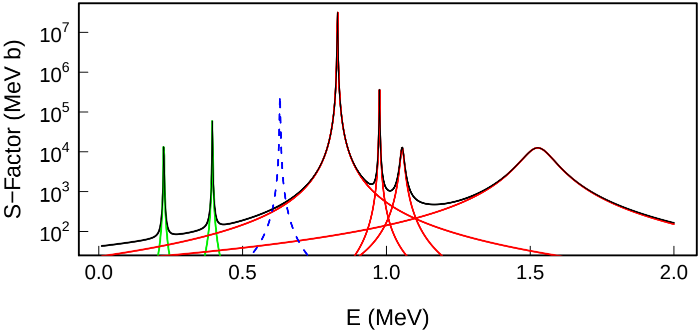
A Fictional Example

^{22}Ri+α



- **Directly Measured Resonances**
  - $E_r^{\text{lab}} = 830$ keV $J^\pi = 2^+$
    $\Gamma_\alpha = 2.8 \times 10^{-5}$ eV, $\Gamma_\gamma = 3.0(15)$ eV,
    $\Gamma_n = 2.5(17) \times 10^2$ eV
- **Indirectly Measured Resonances**
  - $E_r^{\text{lab}} = 226$ keV $J^\pi = 1^-$
    $S_\alpha = 1.9 \times 10^{-2}$, $\Gamma_\gamma = 0.72(18)$ eV
  - $E_r^{\text{lab}} = 395$ keV $J^\pi = 1^-$
    $S_\alpha = 2.8 \times 10^{-3}$, $\Gamma_\gamma = 1.9(3)$ eV
- **Upper Limit Resonances**
  - $E_r^{\text{lab}} = 630$ keV $J^\pi = 1^-$
    $\omega\gamma < 6 \times 10^{-3}$ neV
    $\Gamma_\gamma = 3.0(15)$ eV,
    $\Gamma_n = 1.7(8) \times 10^3$ eV,
    $\Gamma_\alpha < 1.7 \times 10^{-9}$ eV

A Fictional Example



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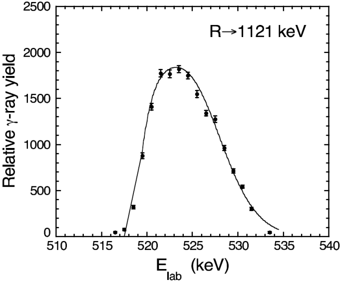
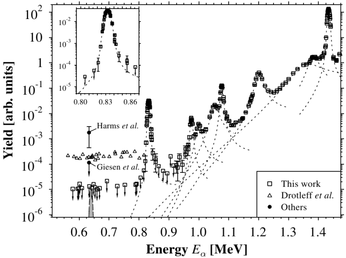
Directly Measured Resonances



Fox, C. *et al.*, Phys. Rev. C 71 (2005) 055801



Jaeger, M. *et al.*, Phys. Rev. Lett. 87 (2001) 202501

- **Narrow Resonances**
  - Thick targets
  - Precise resonance energy
  - Resonance strength $\omega\gamma$

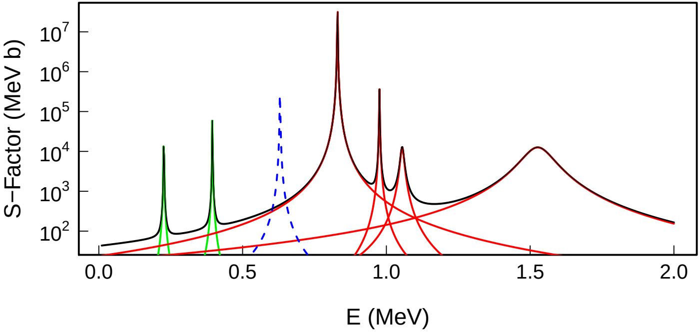
$$\omega\gamma = \frac{2\varepsilon_{\text{eff}}}{\lambda_r^2}\frac{N_{\text{max}}}{N_b B \eta W}$$

  - Central Limit Theorem
    Multiplication of quantities leads to Lognormal uncertainties.
- **Wide Resonances**
  - Thin targets
  - Total resonance width Γ
  - Resonance strength $\omega\gamma$

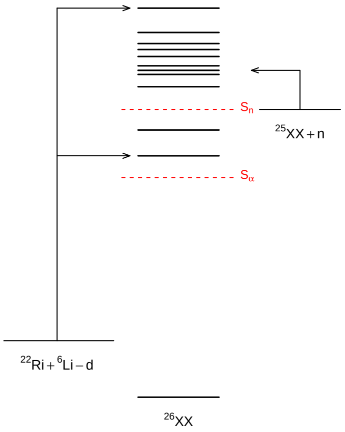
Cross Section

$$\sigma \sim \frac{\Gamma_a(E)\Gamma_b(E)}{(E_r - E)^2 + \Gamma(E)^2/4}$$

$$\Gamma(E) \sim P_c(E)\theta^2 \qquad \Gamma(E) = \Gamma(E_r)\frac{P_c(E)}{P_c(E_r)}$$



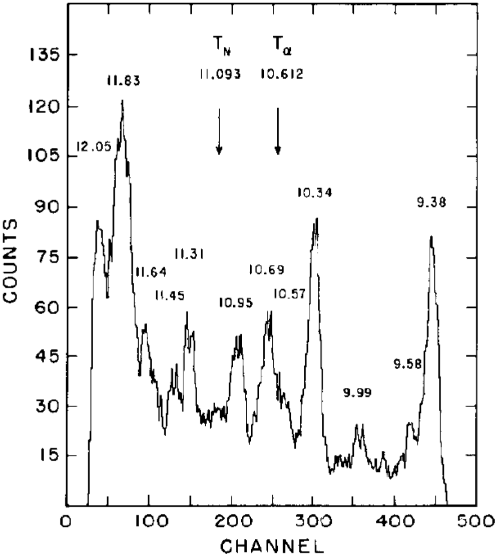
Indirectly Measured Resonances



- Transfer Reactions
  - Γ_α (S-factors, ANCs etc.)
  - Energies
  - Quantum Numbers
- Neutron Capture
  - Γ_n
  - Energies
  - Branching Ratios
- Photoexcitation
  - Γ_γ
  - Energies
  - Branching Ratios

- Indirect methods used mostly for low energy resonances
- Energy uncertainty can be large

Indirectly Measured Resonances

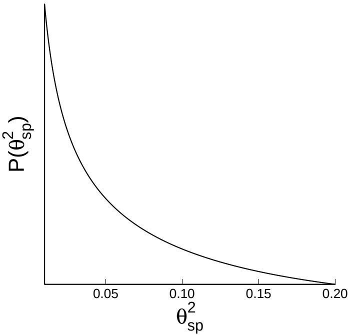


Example: ^{22}Ne(^{6}Li,d)^{26}Mg

- (^{6}Li,d) reaction populates states either side of α-particle threshold
- Large energy uncertainties
- Upon subtracting S_α, one obtains resonance energy with finite probability of negative energy (sub-threshold resonance)
- Central Limit Theorem *Addition of quantities leads to Gaussian uncertainties.*

U. Giesen *et al.*, Nucl. Phys. A 561 (1993) 95 – 111

Upper Limit Resonances



- Random matrix theory predicts that dimensionless reduced widths (θ^2_{sp}) should be distributed *locally* according to a Porter-Thomas distribution

$$P(\theta^2) = \begin{cases} \frac{c}{\sqrt{\theta^2}} e^{-\theta^2/(2\langle\theta^2\rangle)} & \text{if } \theta^2 \leq \theta^2_{ul} \\ 0 & \text{if } \theta^2 > \theta^2_{ul} \end{cases}$$

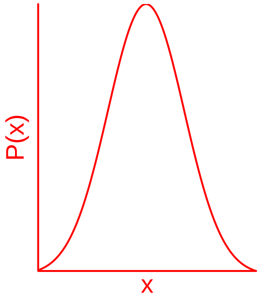
- To estimate $\langle\theta^2\rangle$ for $A = 20 - 40$
  - 360 α-particle widths
    $\langle\theta^2_\alpha\rangle = 0.010$
  - 1127 proton widths
    $\langle\theta^2_p\rangle = 0.0045$
- Nuclear theory and experiments are required

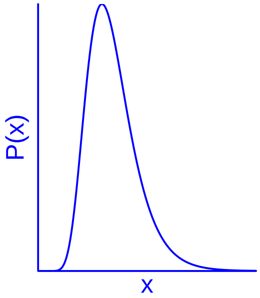
Reaction Rate

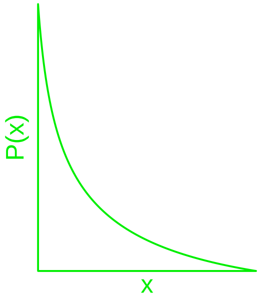
Reaction Rate per Particle Pair

$$\langle \sigma v \rangle = \sqrt{\frac{8}{\pi\mu}} \frac{1}{(kT)^{3/2}} \int_0^\infty E\sigma(E) e^{-E/kT} dE$$

E_r	$\omega\gamma$	$S, S'S''$	Γ_a	Γ_{UL}	$\langle \sigma v \rangle$
Gaussian	Lognormal	Lognormal	Lognormal	Porter-Thomas	Lognormal



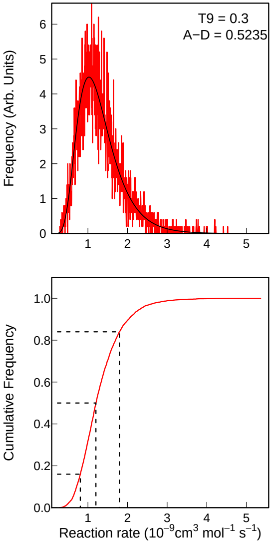




Putting it all Together

```
22Ri(a,g)26XX
******************************************************************************************
2               ! Zproj
12              ! Ztarget
0               ! Zexitparticle (=0 when only 2 channels open)
4.003           ! Aproj
21.991          ! Atarget
1.009           ! Aexitparticle (=0 when only 2 channels open)
0.0             ! Jproj
0.0             ! Jtarget
0.5             ! Jexitparticle (=0 when only 2 channels open)
10614.79        ! projectile separation energy (keV)
11093.08        ! exit particle separation energy (=0 when only 2 channels open)
1.25            ! Radius parameter R0 (fm)
2               ! Gamma-ray channel number (=2 if ejectile is a g-ray; =3 otherwise)
******************************************************************************************
1.0             ! Minimum energy for numerical integration (keV)
5000            ! Number of random samples (>5000 for better statistics)
0               ! =0 for rate output at all temperatures; =NT for rate output at selected temperatures
**************************************************************************************** ********
Nonresonant Contribution
S(keVb)  S'(b)   S''(b/keV)   fracErr   Cutoff Energy (keV)
0.0      0.0     0.0          0.0       0.0
0.0      0.0     0.0          0.0       0.0
******************************************************************************************
Resonant Contribution
Note: G1 = entrance channel, G2 = exit channel, G3 = spectator channel !! Ecm, Exf in (keV); wg, Gx in (eV) !!
Note: if Er<0, theta^2=C2S*theta_sp^2 must be entered instead of entrance channel partial width
Ecm      DEcm    wg      Dwg     J   G1        DG1       L1  G2   DG2  L2  G3       DG3      L3  Exf  Int
191.08   0.15    0       0       1   1.25e-23  0.50e-23  1   0.7  0.2  1   0        0        0   0    0
334.31   0.1     0       0       1   1.20e-9   0.50e-9   1   1.9  0.3  1   0        0        0   0    0
703.78   2.11    0       0       2   2.8e-5    0.5e-5    2   3.0  1.5  1   2.5e2    1.7e2    1   0    1
826.04   0.19    0       0       4   3.78e-6   4.44e-7   4   3.0  1.5  1   1.47e3   8.0e1    2   0    1
893.31   0.90    0       0       1   1.17e-4   2.0e-5    1   3.0  1.5  1   1.27e4   2.5e3    1   0    1
1294.6   1.20    0       0       2   2.80e-6   0.1e-6    2   2.3  1.0  1   1.10e5   0.05e5   1   0    1
******************************************************************************************
Upper Limits of Resonances
Note: enter partial width upper limit by chosing non-zero value for PT, where PT=<theta^2> for particles and...
Note: ...PT=<B> for g-rays [enter: "upper_limit 0.0"]; for each resonance: # upper limits < # open channels!
Ecm      DEcm    Jr   G1        DG1  L1  PT    G2      DG2     L2  PT  G3      DG3     L3  PT  Exf   Int
533.1    0.8     1    1.7e-9    0    1   0.01  3.0     1.5     1   0   1.7e3   0.8e3   1   0   0     0
******************************************************************************************
```

Rate Distribution



- Distributions of rates are calculated
- Useful statistical parameters
  - Median
  - 1σ uncertainties (16th and 84th percentiles)
- Entire distribution of rates described by *lognormal distribution*

$$\mu = \ln(E[x]) - \frac{1}{2}\ln\left(1 + \frac{V[x]}{E[x]^2}\right), \quad \sigma = \sqrt{\ln\left(1 + \frac{V[x]}{E[x]^2}\right)}$$

- Lognormal distribution is an assumption
- Anderson-Darling statistic describes how well distribution is fit by the lognormal

$$t_{AD} = -n - \sum_{i=1}^{n} \frac{2i-1}{n}\left(\ln F(y_i) + \ln\left[1 - F(y_{n+1-i})\right]\right)$$

- $t_{AD} < 40$ corresponds to good *visual* agreement

Stephens, M.A., J. Am. Stat. Assoc. 69 (1973) 74

Rate Presentation

T (GK)	Low rate	Median rate	High rate	lognormal μ	lognormal σ	A-D
0.100	2.47×10^{-20}	3.67×10^{-20}	5.48×10^{-20}	$-4.475\times10^{+01}$	4.06×10^{-01}	5.29×10^{-01}
0.110	7.28×10^{-19}	1.08×10^{-18}	1.62×10^{-18}	$-4.137\times10^{+01}$	4.06×10^{-01}	5.29×10^{-01}
0.120	1.21×10^{-17}	1.79×10^{-17}	2.68×10^{-17}	$-3.856\times10^{+01}$	4.06×10^{-01}	5.30×10^{-01}
0.130	1.29×10^{-16}	1.91×10^{-16}	2.86×10^{-16}	$-3.619\times10^{+01}$	4.06×10^{-01}	5.30×10^{-01}
0.140	9.72×10^{-16}	1.44×10^{-15}	2.16×10^{-15}	$-3.417\times10^{+01}$	4.06×10^{-01}	5.30×10^{-01}
0.150	5.56×10^{-15}	8.25×10^{-15}	1.23×10^{-14}	$-3.243\times10^{+01}$	4.06×10^{-01}	5.30×10^{-01}
0.160	2.54×10^{-14}	3.77×10^{-14}	5.64×10^{-14}	$-3.091\times10^{+01}$	4.06×10^{-01}	5.29×10^{-01}
0.180	3.15×10^{-13}	4.68×10^{-13}	6.98×10^{-13}	$-2.839\times10^{+01}$	4.06×10^{-01}	5.29×10^{-01}
0.200	2.32×10^{-12}	3.45×10^{-12}	5.15×10^{-12}	$-2.639\times10^{+01}$	4.06×10^{-01}	5.29×10^{-01}
0.250	8.05×10^{-11}	1.19×10^{-10}	1.78×10^{-10}	$-2.285\times10^{+01}$	4.06×10^{-01}	5.28×10^{-01}
0.300	8.14×10^{-10}	1.21×10^{-09}	1.80×10^{-09}	$-2.053\times10^{+01}$	4.06×10^{-01}	5.23×10^{-01}
0.350	4.11×10^{-09}	6.10×10^{-09}	9.08×10^{-09}	$-1.891\times10^{+01}$	4.05×10^{-01}	4.96×10^{-01}
0.400	1.37×10^{-08}	2.02×10^{-08}	3.00×10^{-08}	$-1.772\times10^{+01}$	4.00×10^{-01}	4.35×10^{-01}
0.450	3.55×10^{-08}	5.14×10^{-08}	7.58×10^{-08}	$-1.678\times10^{+01}$	3.88×10^{-01}	4.13×10^{-01}
0.500	7.85×10^{-08}	1.12×10^{-07}	1.63×10^{-07}	$-1.600\times10^{+01}$	3.74×10^{-01}	4.65×10^{-01}
0.600	2.89×10^{-07}	4.16×10^{-07}	6.16×10^{-07}	$-1.468\times10^{+01}$	3.89×10^{-01}	$1.77\times10^{+00}$
0.700	8.29×10^{-07}	1.26×10^{-06}	2.06×10^{-06}	$-1.355\times10^{+01}$	4.74×10^{-01}	$1.10\times10^{+01}$
0.800	2.00×10^{-06}	3.29×10^{-06}	5.94×10^{-06}	$-1.258\times10^{+01}$	5.60×10^{-01}	$1.31\times10^{+01}$
0.900	4.26×10^{-06}	7.48×10^{-06}	1.44×10^{-05}	$-1.176\times10^{+01}$	6.18×10^{-01}	$1.00\times10^{+01}$
1.000	8.21×10^{-06}	1.51×10^{-05}	2.98×10^{-05}	$-1.106\times10^{+01}$	6.48×10^{-01}	$7.46\times10^{+00}$

Conclusions

- Statistically meaningful uncertainties of thermonuclear nuclear reaction rates formulated
- Treatment of upper limits based on nuclear physics theory
- Flexible method allows for reasonable uncertainty assignments
  - **Energies:** Gaussian
  - **Resonance Strengths:** Lognormal
  - **Partial Widths:** Lognormal
  - **Upper Limits:** Porter-Thomas Distribution
- Final uncertainties can be presented as lognormal parameters
- Allows for full Monte Carlo sensitivity studies to be performed

- See:
  Longland, R. *et al.*, Nucl. Phys. A 841 (2010) 1–30
  Iliadis, C. *et al.*, Nucl. Phys. A 841 (2010) 31–250
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  - US Department of Energy under Contract No. DE-FG02-97ER41041.

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