Nuclear Reactions for Applications

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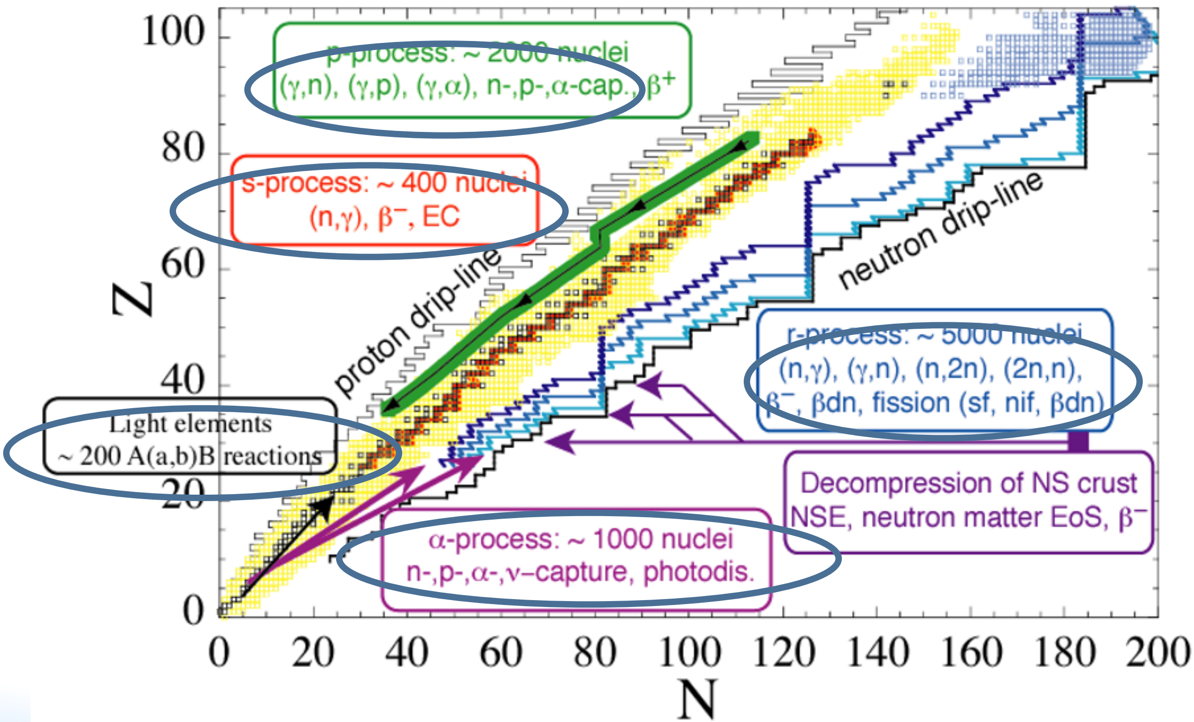
General

- Nuclear reactions are the means by which we study nuclear properties- both structure and dynamics
  - Inelastic scattering to low-lying states to extract spins
  - Reactions in the resonance region to study resonances and spins-parities
  - Transfer and knockout reactions
  - Coulomb excitation
  - Heavy ion reactions – fusion evaporation reactions to study structure properties of neutron-deficient nuclei
  - Fission and deep inelastic scattering to study nuclear structure or neutron-rich nuclei
  - Photonuclear reactions and Nuclear Resonance Fluoresence to study the E/M response of the nucleus (GDR, pygmy, etc)

General cont’d

- Nuclear reactions are studied because we want to know how ions interact with nuclear matter and how to produce nuclear species at different energies and angles
  - Nuclear reactor inventories – production of neutrons, fission products, delayed neutrons
  - Fusion plasma erosion of structural material
  - Surface and bulk analysis of materials
  - Production of radioisotopes for medical applications
  - Radiation transport in materials
  - Production of nuclei in the universe: nucleosynthesis (astrophysical reaction rates) etc

Example: Nucleosynthesis data needs



General cont'd

- Nuclear reactions are studied because we want to know how ions interact with nuclear matter and how to produce nuclear species at different energies and angles

Applications:

Projectiles: γ, n, p, d, t, ^{3}He, α, fission light ions (Be, Li, C)

Incident energies: up to ~200 MeV

  - Production of nuclei in the universe (astrophysical reaction rates) etc

Nuclear reactions

$$a + A \rightarrow b + B$$

Target nucleus

$$A(a,b)B$$

Residual nucleus-
Undetected part

Projectile-
Incident beam

Ejectile-
Detected particle

Q-value = masses (before) – masses (after)

$$= M_a + M_A - M_B - M_b$$

Q-value > 0 : exothermic
Q-value < 0 : endothermic
Q = 0 : elastic scattering

Thresholds of reaction channels

Depend on Q-value

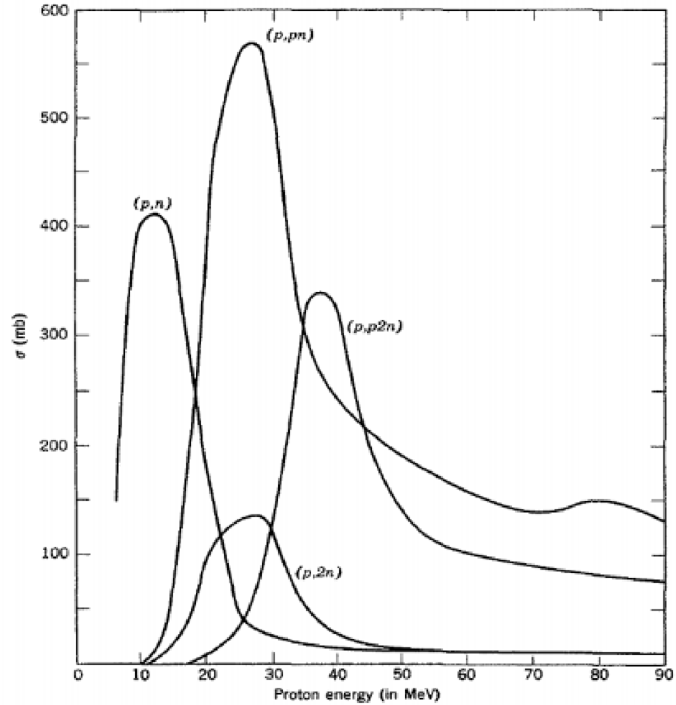
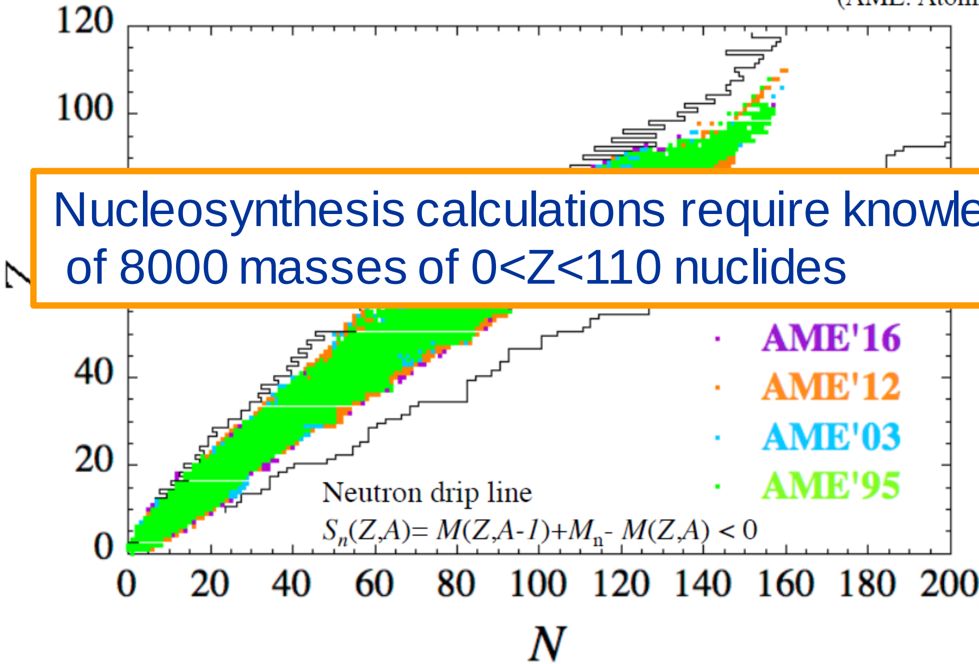


Fig. 4-5 Excitation functions for proton-induced reactions on ^{63}Cu. [From J. W. Meadows, *Phys. Rev.* **91**, 885 (1953).]

Masses

AME 2016 (Wang et al, CJP 41 (2017)):
2498 experimentally known masses + 938 extrapolated = 3436 recommended masses

(AME: Atomic Mass Evaluation)

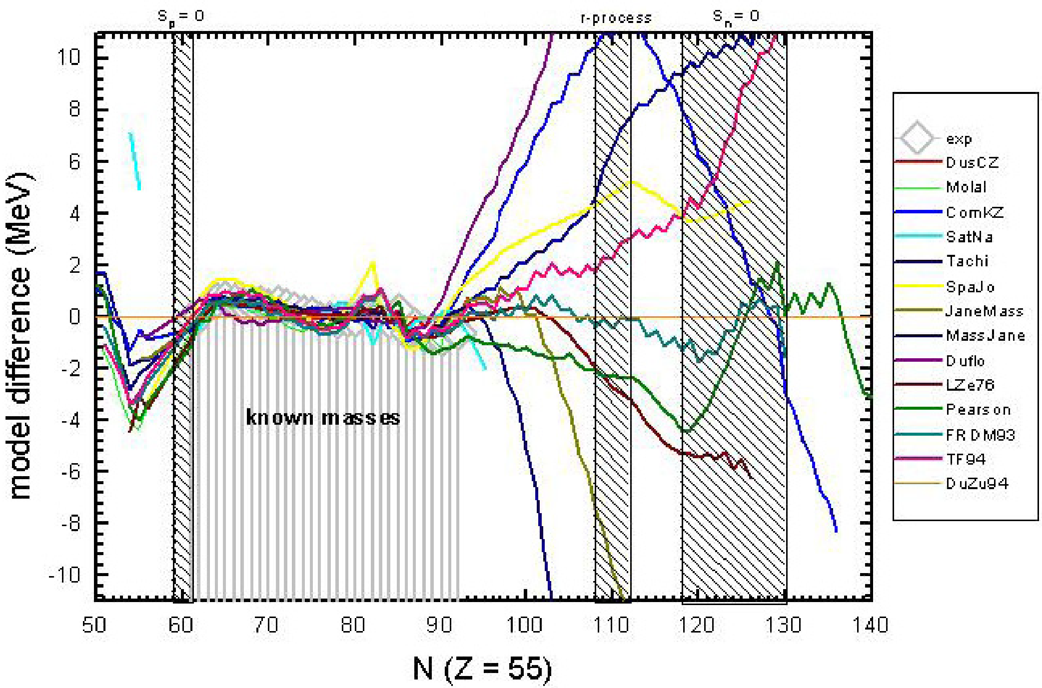


Nucleosynthesis calculations require knowledge of 8000 masses of 0<Z<110 nuclides

Masses: global models

- **Macroscopic-Microscopic Approaches**
  - Liquid drop model (Myers & Swiateki 1966)
  - Droplet model (Hilf et al. 1976)
  - FRDM model (Moller et al. 1995, 2012)
  - KUTY model (Koura et al. 2000)
  - Weizsäcker-Skyrme model (Wang et al. 2011)
- **Approximation to Microscopic models**
  - Shell model (Duflo & Zuker 1995)
  - ETFSI model (Aboussir et al. 1995)
- **Mean Field Model**
  - Hartree-Fock-BCS model (2000)
  - Hartree-Fock-Bogolyubov model (2010)
  - Relativistic Hartree-Bogolyubov

Global mass models: extrapolation to unknown region



Cross section

- Probability of a projectile to ‘hit’ a target nucleus and interact with it (scatter, break up, transfer a particle etc)
- Formal definition (Fermi Golden Rule)

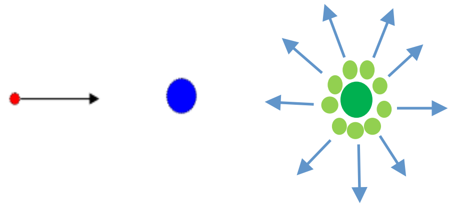
$$\text{Probability} = n \bullet x \bullet \sigma$$

n = # nuclei per volume; x = thickness; σ = effective area of nucleus for reaction

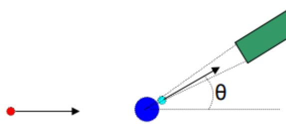
- σ (units = 10^{-24} cm^2 or 1 barn) – in nuclear physics mb (10^{-3} b) or µb (10^{-6} b)

Types of measured cross sections

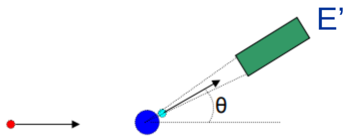
- Total cross sections σ_T (in 4π)



- Angular distribution $d\sigma/d\Omega$ (in $d\Omega$)



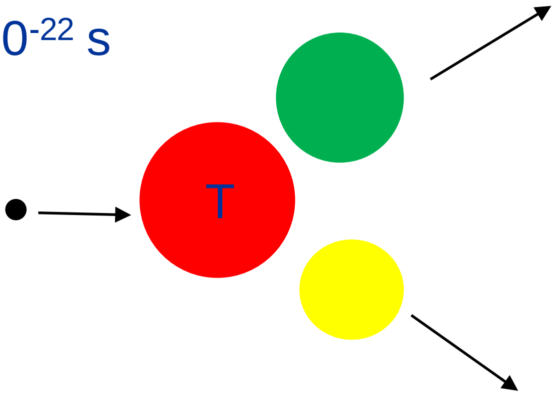
- Double-differential cross sections $d^2\sigma/dEd\Omega$ (emission spectrum: in $d\Omega$ with E')



Reaction mechanisms

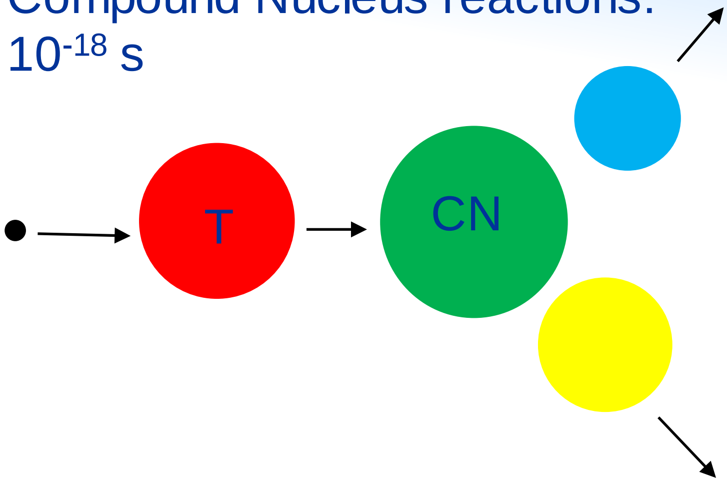
Depending on incident energy

Direct reactions:
10^{-22} s



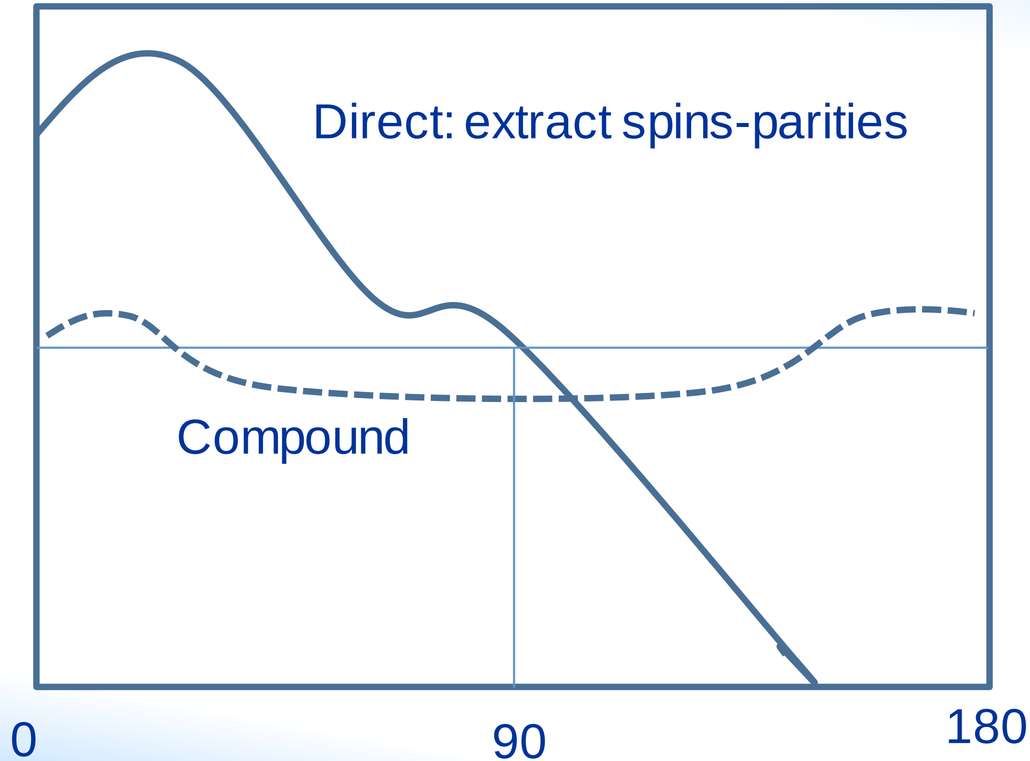
- Elastic scattering
- Inelastic scattering
- Transfer reactions (stripping, pickup)
- Knock-out
- Capture
- Break-up

Compound Nucleus reactions:
10^{-18} s



- Resonance scattering
- Evaporation
- Fission

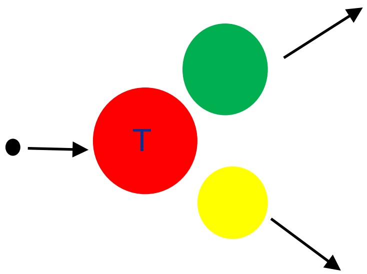
Angular distributions dσ/dΩ



Reaction mechanisms I

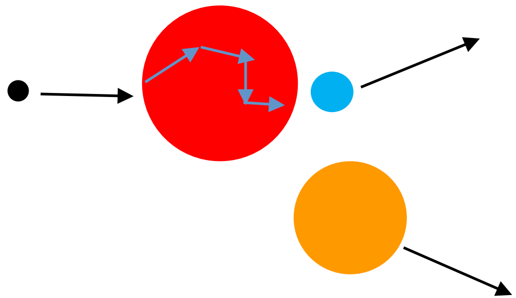
Depending on incident energy

Direct reactions: 10^{-22} s



- Elastic scattering
- Inelastic scattering
- Capture
- Transfer reactions (stripping, pickup)
- Knock-out
- Break-up

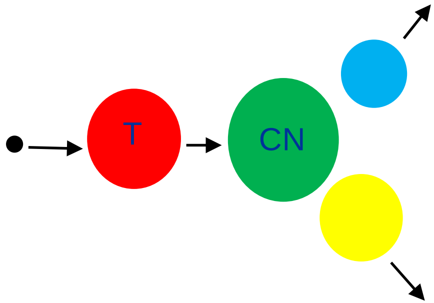
Preequilibrium reactions



- Inelastic scattering
- Transfer reactions (stripping, pickup)
- Knock-out
- HI reactions

Above ~ 10 MeV Incident energy

Compound Nucleus reactions: 10^{-18} s

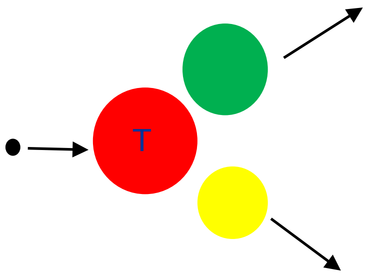


- Resonance scattering
- Evaporation (incl. radiative capture)
- Fission

Reaction mechanisms II

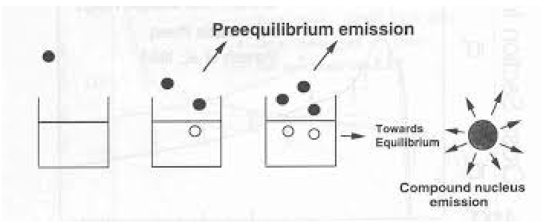
Depending on incident energy

Direct reactions: 10^{-22} s



- Elastic scattering
- Inelastic scattering
- Capture
- Transfer reactions (stripping, pickup)
- Knock-out
- Break-up

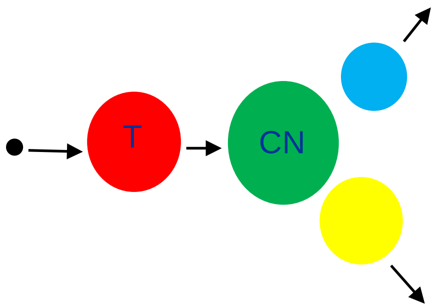
Preequilibrium reactions: exciton model



- Inelastic scattering
- Transfer reactions (stripping, pickup)
- Knock-out

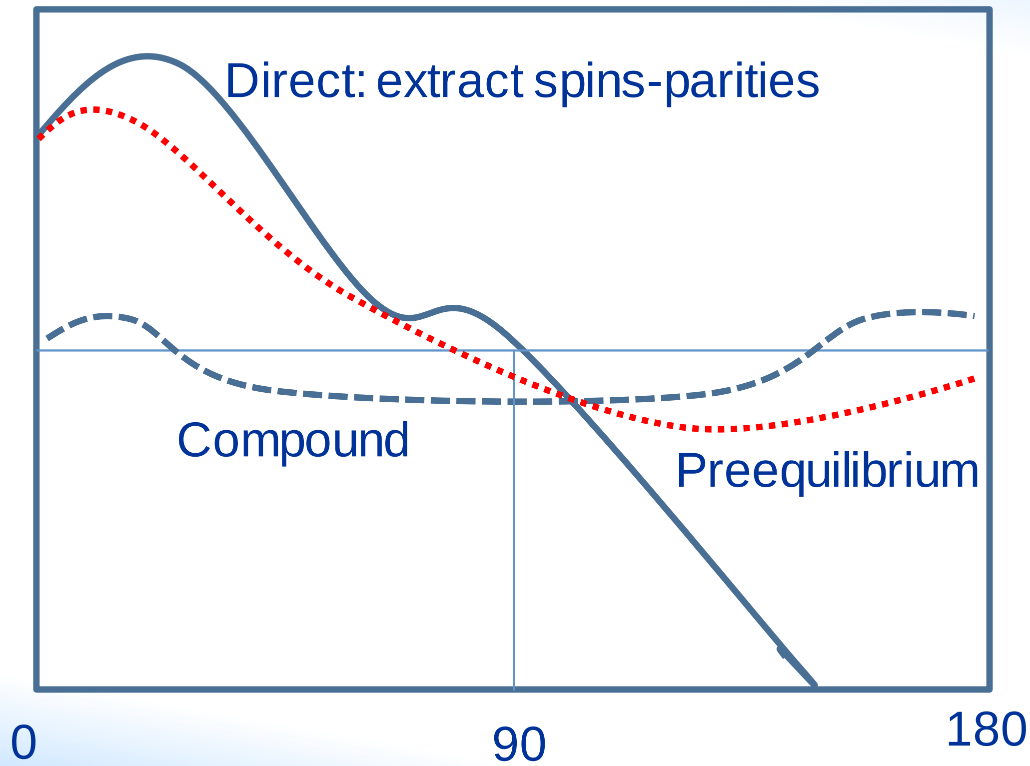
Above ~ 10 MeV

Compound Nucleus reactions: 10^{-18} s

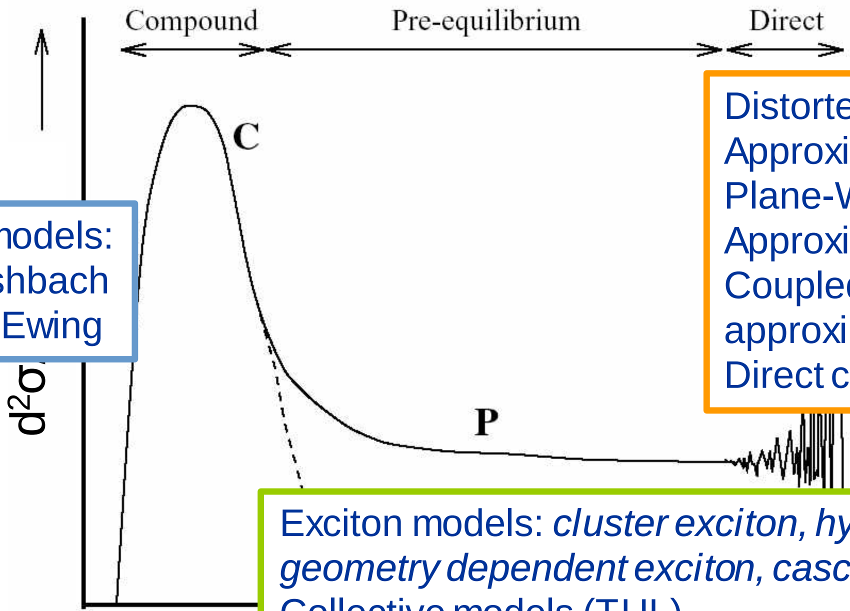


- Resonance scattering
- Evaporation (incl. radiative capture)
- Fission

Angular distributions dσ/dΩ



Reaction Models



Statistical models:
Hauser Feshbach
Weisskopf-Ewing

Distorted-Wave Born Approximation (DWBA)
Plane-Wave Impulse Approximation (PWIA)-HE
Coupled-Channels approximations
Direct capture models

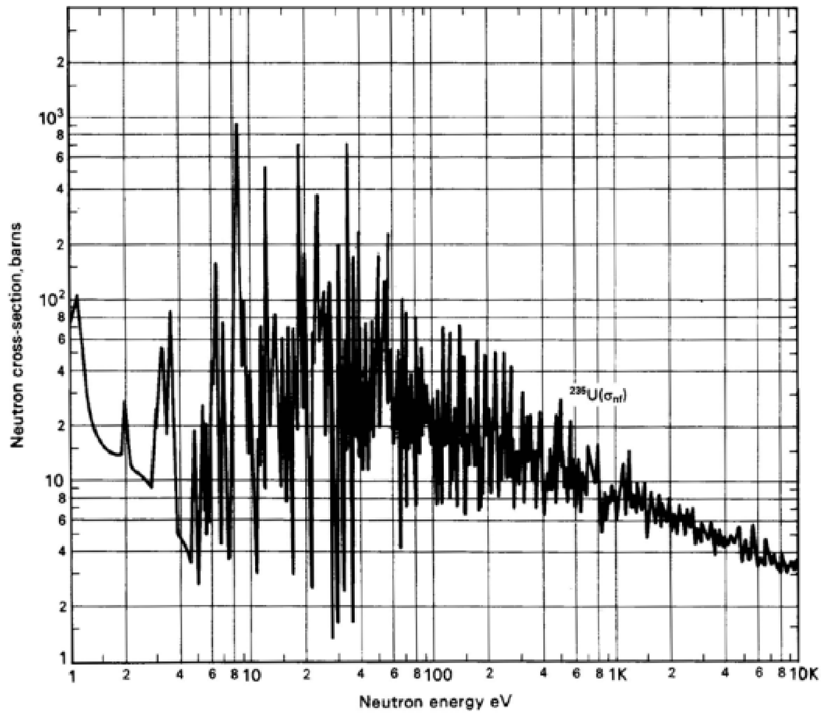
Exciton models: *cluster exciton, hybrid exciton, geometry dependent exciton, cascade exciton*
Collective models (TUL)
QM model (FKK)

Slow neutron reactions

Cross sections for neutrons at thermal energies (0.025 eV) follow 1/v law

Coulomb barrier hinders proton-induced reactions at very low energies (<1 MeV)

Problem for Nuclear Astrophysics: Cross sections are extrapolated

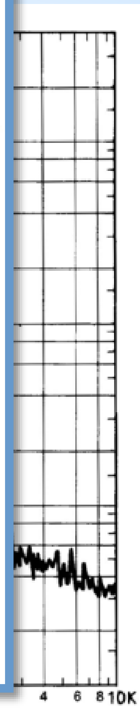


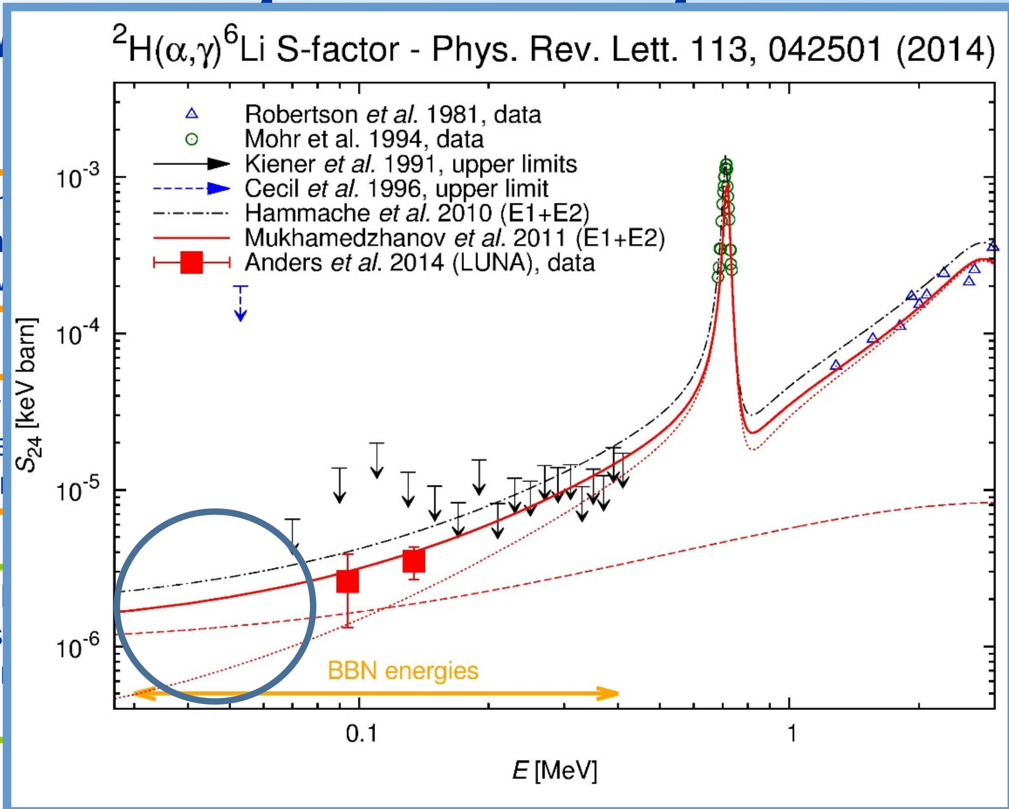
Slow

Cross sectio
at thermal en
follow 1/v law

Coulomb bar
proton-induce
at very low e

Problem for
Astrophysics
Cross sectio
extrapolated





Cross section calculations

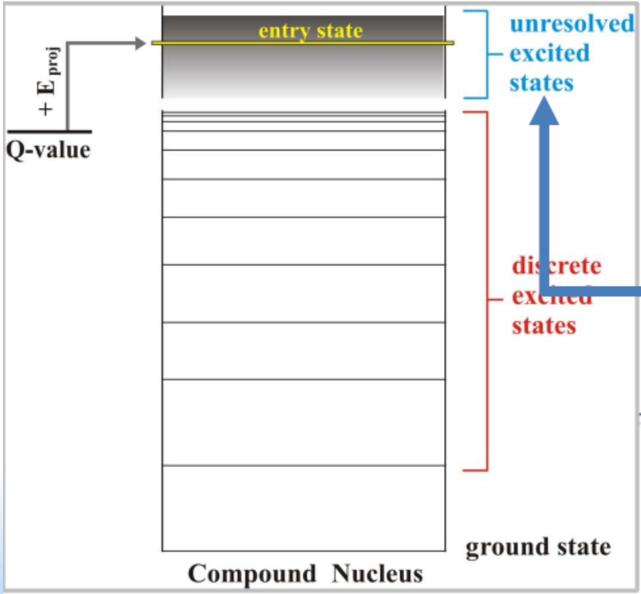
- Depending on incident energy more than one reaction channel may be open
- Use different models to describe reaction channels at different energies
- Models make use of parameters that have to be adjusted to experimental data
- Independent experimental information can be used to constrain the parameters

Compound nucleus reactions

Statistical model: excitation to overlapping states

$\alpha + A \rightarrow C^* \rightarrow b + B$

$$\sigma_{bB} = \frac{\pi\lambda^2}{(2J_\alpha + 1)(2J_A + 1)} \sum_{J^\pi} (2J_C + 1)\, T_{\alpha A}^{J^\pi} \frac{T_{bB}^{J^\pi}}{\sum_i T_i^{J^\pi}}$$



$T_{\alpha A}$

probability that **α** will cross the surface of **A** to form a compound state of **C** having spin ***J***

T_{bB}

probability that **b** escapes from a state of the compound nucleus **C** with spin ***J***

sum of probabilities over all exit channels ***i***

T's averaged over Nuclear Level Densities

$$\bar{T}_{\alpha A} = \sum_I \int \rho(E_\alpha, I)\, T_{\alpha A}^I(E_\alpha)\, dE_\alpha$$

Ingredients of HF cross sections

IAEA

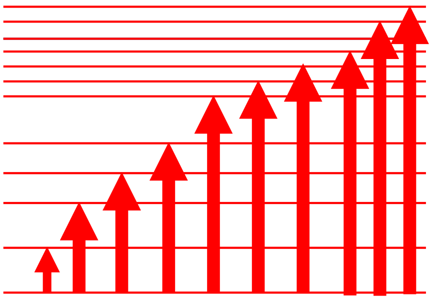
- Particle entrance/exit channels: $a + A$
  transmission coefficients T_{aA} are obtained by solving scattering of projectile a off target A using an Optical Model Potential (OMP):
  $U = V_c + V + i \cdot W$ (T's are related to scatt. amplitudes)

- Photon exit channel: $\gamma + A$
  transmission coefficient $T_{\gamma A}$ is obtained from Giant Resonances Strength Function (γSF) assuming E1/M1 transitions are important

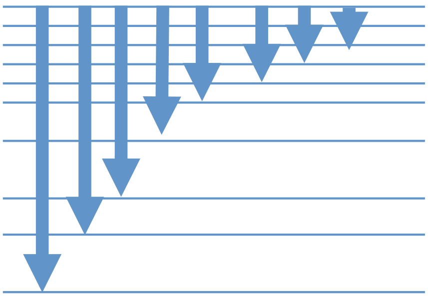
- For excitations to phase space where levels are strongly overlapping and un-resolved: Nuclear Level Density (NLD) formulas are used to describe number of states per E and J

- Ground-state properties: masses, deformations, density distributions, single-particle level schemes are obtained from nuclear models

Photon Strength Function



(E_0, J_0, π_0)



(E_f, J_f, π_f)

From (γ,abs), (γ,xn):

$$\sigma(E_\gamma) = 3E_\gamma(\pi\hbar c)^2 \vec{\boldsymbol{f}}(\boldsymbol{E_\gamma})$$

From (γ,γ), charged-particle reactions, average resonance captures

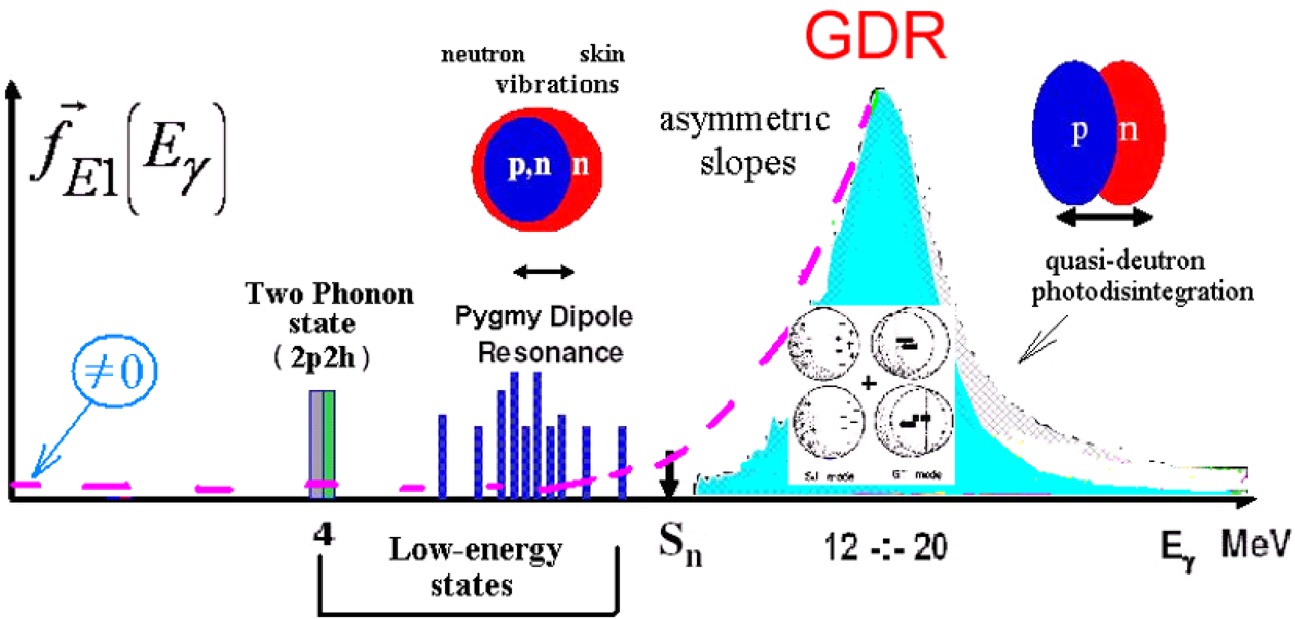
$$\overleftarrow{\boldsymbol{f}}(\boldsymbol{E_\gamma}, \boldsymbol{T}) \rightarrow \boldsymbol{\Gamma}(\boldsymbol{E_\gamma}, \boldsymbol{T})$$

Temperature

Photon Strength Function

Dipole electric gamma-transitions are dominant ones, if they take place together with transitions of other multipolarities and types

Nuclear states excited by E1 field



Empirical Photon Strength Functions

Standard Lorentzian (SLO) *Brink(1955)& Axel(1962)*

Depressed Lorentzian (DLO) *Lane&Lynn(1960)*

Fermi liquid model (KFM) *Kadmensky, Markushev, Furman(1983)*

Enhanced Generalized Lorentzian (EGLO) *Kopecky& Uhl(1993)*

Hybrid model (GH) *Goriely (1998)*

Modified Lorentzian model (MLO) *Plujko et al (1999)*

Generalized Fermi liquid model (GFL) *Mughabghab&Dunford (2000)*

Triple (triaxial) Lorentzian model (TL) *Junghans et al (2008)*

Empirical Photon Strength Functions

Standard Lorentzian (SLO) *Bri*

Depressed Lorentzian (DLO) *L*

Fermi liquid model (KFM) *Kad*

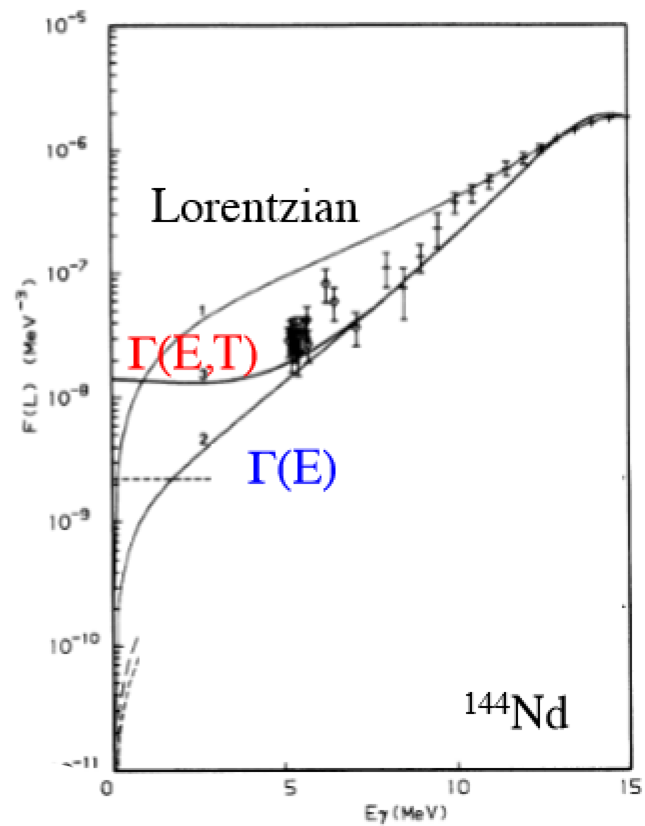
Enhanced Generalized Lorentzi

Hybrid model (GH) *Goriely (19*

Modified Lorentzian model (M

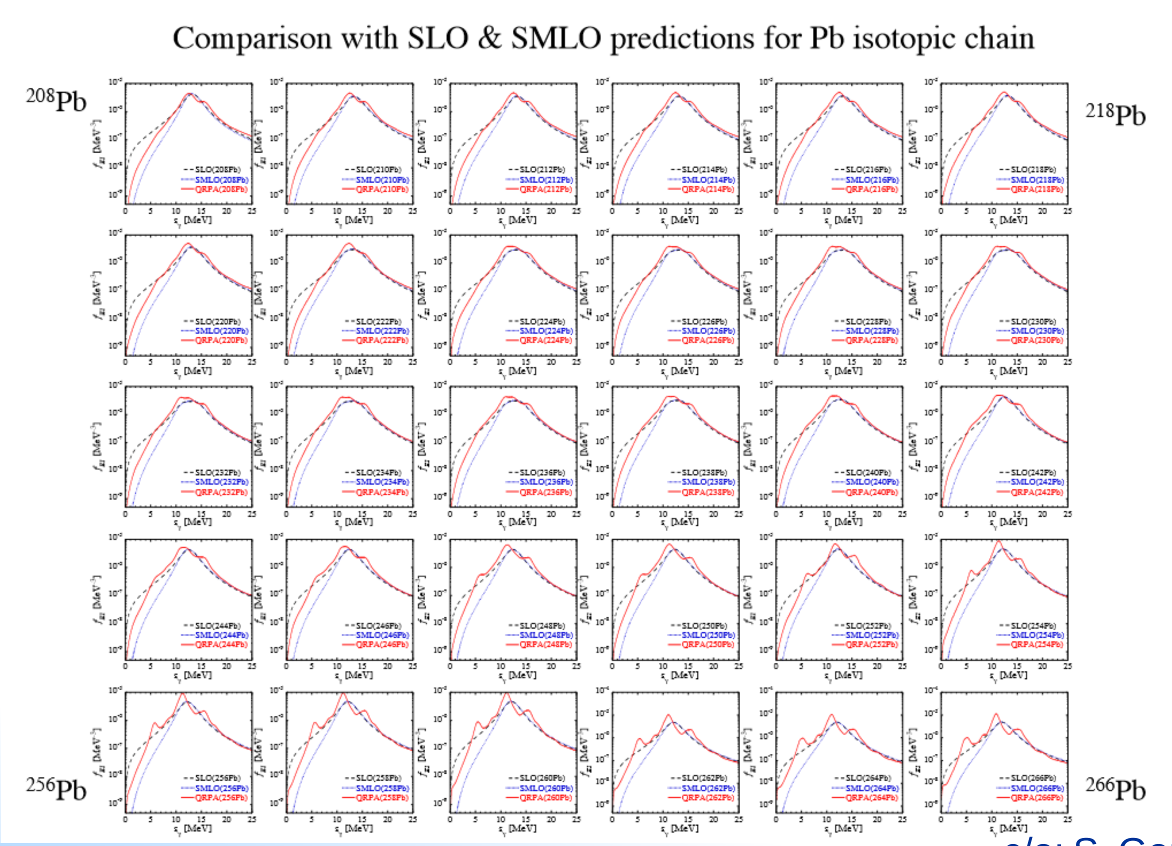
Generalized Fermi liquid model

Triple (triaxial) Lorentzian mod



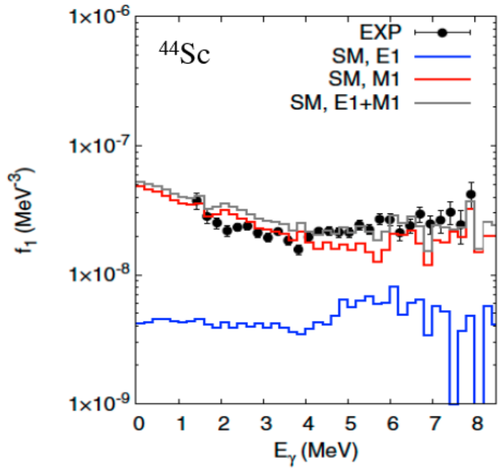
Semi-microscopic PSF

HFB+ QRPA (Goriely et al.)



c/o: S. Goriely

Low-energy limit of Photon Strength Functions



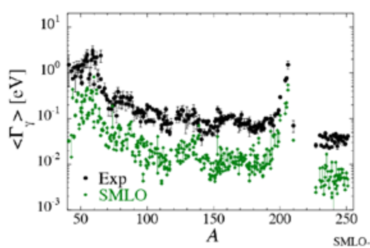
Non-zero limit of the *E1* strength at $\varepsilon_\gamma \to 0$

Upbend of the *M1* strength at $\varepsilon_\gamma \to 0$

Impact on Total Radiative Capture Width $<\Gamma_\gamma>$

SMLO E1 strength + RIPL-3 M1 strength and its impact on the radiative width $<\Gamma_\gamma>$

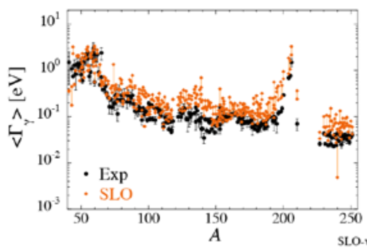
$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



where error bars on predictions are obtained with different NLD models

SLO E1 strength + RIPL-3 M1 strength and its impact on the radiative width $<\Gamma_\gamma>$

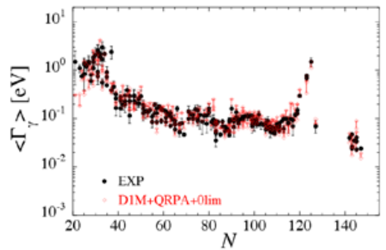
$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



where error bars on predictions are obtained with different NLD models

D1M+QRPA E1 & M1 strength + non-zero limit and its impact on the radiative width $<\Gamma_\gamma>$

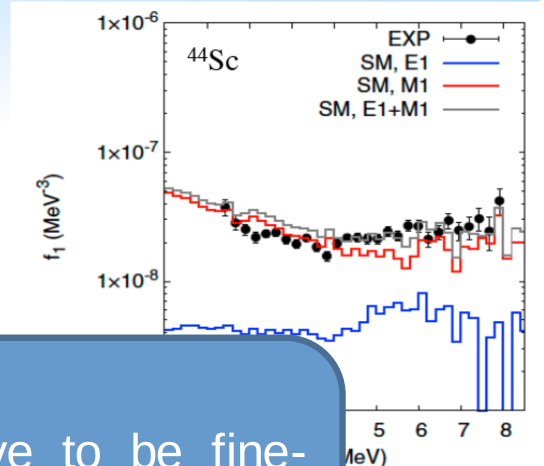
$$\langle \Gamma_\gamma \rangle = \frac{D_0}{2\pi} \sum_{X,L,J,\pi} \int_0^{S_n+E_n} T_{XL}(\varepsilon_\gamma) \times \rho(S_n + E_n - \varepsilon_\gamma, J, \pi) d\varepsilon_\gamma$$



where error bars on predictions are obtained with different NLD models

c/o: S. Goriely

Low-energy limit of Photon Strength Functions



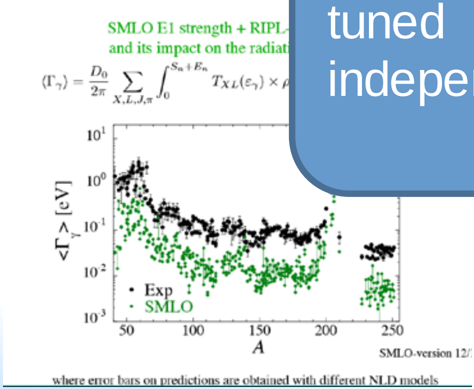
Non-zero limit of the *E1* strength at $\varepsilon_\gamma \rightarrow 0$

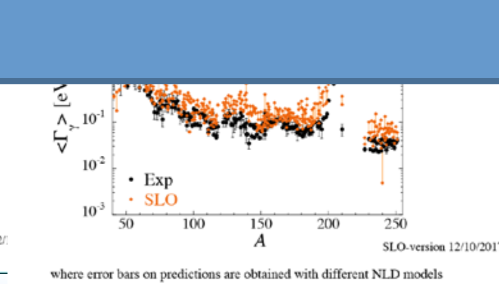
Upbend of the *M1* strength at $\varepsilon_\gamma \rightarrow 0$

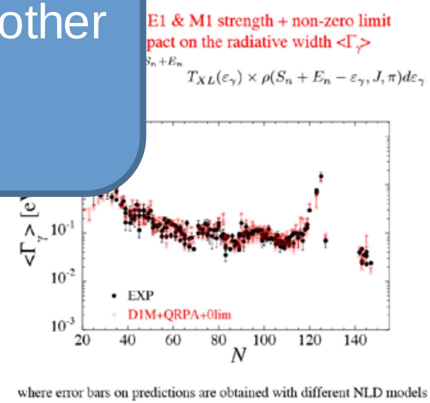
Impact o

Capture

Models of PSFs have to be fine-tuned or tested against other independent data







c/o: S. Goriely

Compound Nucleus: R-matrix theory

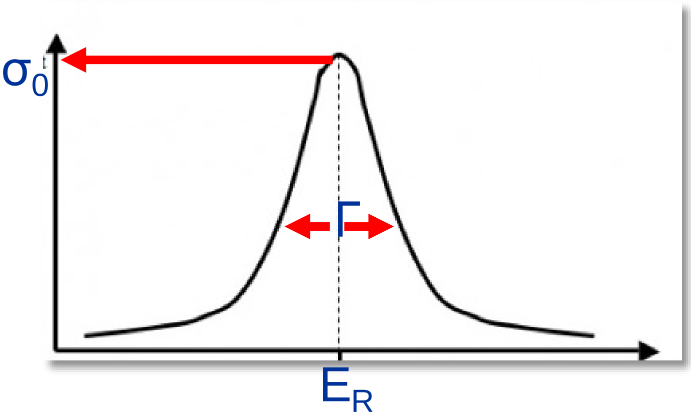
- Nucleus excited to resolved resonance states
- R-matrix theory to describe individual resonances and non-resonant background between them
- Describes the asymptotic wavefunctions outside a fixed radius, R ≥ *a* in terms of pole energies e_p and reduced width amplitudes γ_{np} for each channel n and pole p

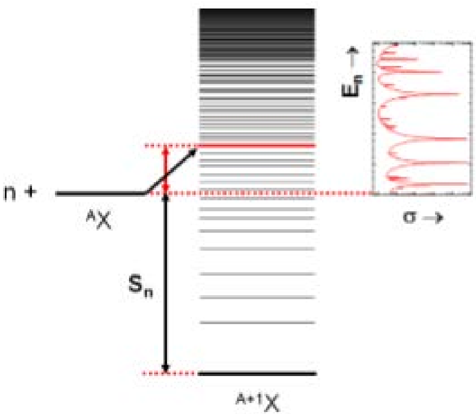
  - e_p taken from nuclear structure (ENSDF) and fitted
  - γ_{np} taken from nuclear structure (ENSDF) and fitted

In practice sum over finite poles

$$\boxed{R_{mn}(E) = \sum_{p=1}^{\infty} \frac{\gamma_{mp}\gamma_{np}}{E-e_p}}$$

Compound nucleus: Resonances





$e_p \rightarrow E_R$
$\gamma_{np} \rightarrow \Gamma$

single resonance:

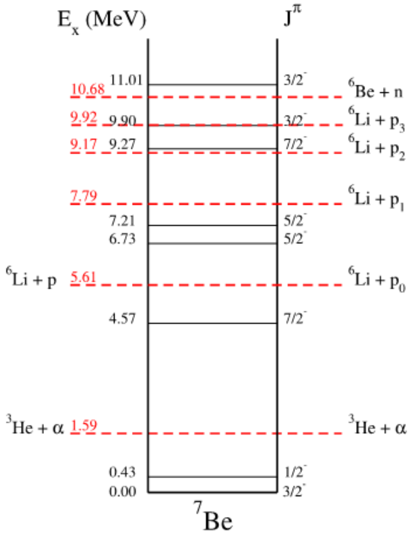
$$\sigma \sim \frac{\Gamma}{(E - E_R)^2 + (\Gamma/2)^2}$$

Level distance: D
Level width Γ:

Resolved: D>Γ
Continuum: D<Γ

R-matrix calculations

Examples: ^4He+^3He elastic scattering with p+^6Li Find R-matrix fit.



Selected data to be fit
up to 8.0 MeV $^7Be^*$ excitation

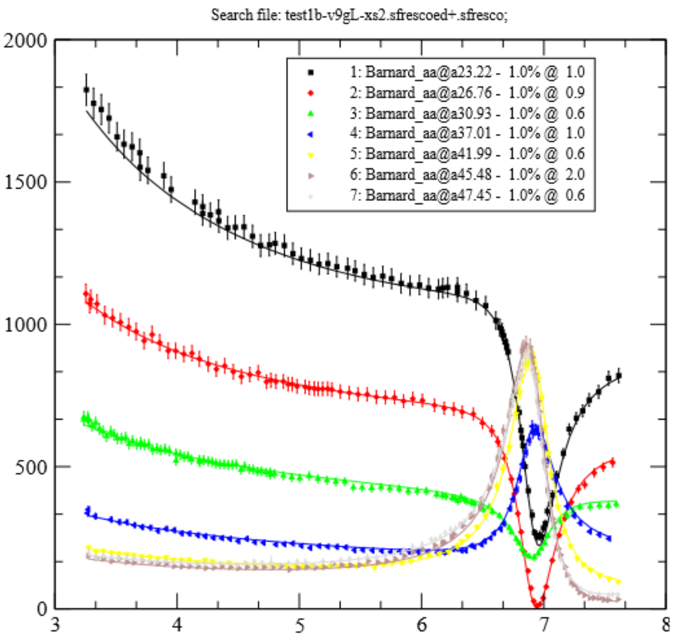
Channels	Data points
(a,a)	1609
(a,p)	120
(p,a)	630
(p,p)	420

Dominant channels: ^4He+^3He and p+^6Li
Next: p_1+$^6Li^*$ (p_1=3^+, p_2=2^+,etc) breakup.

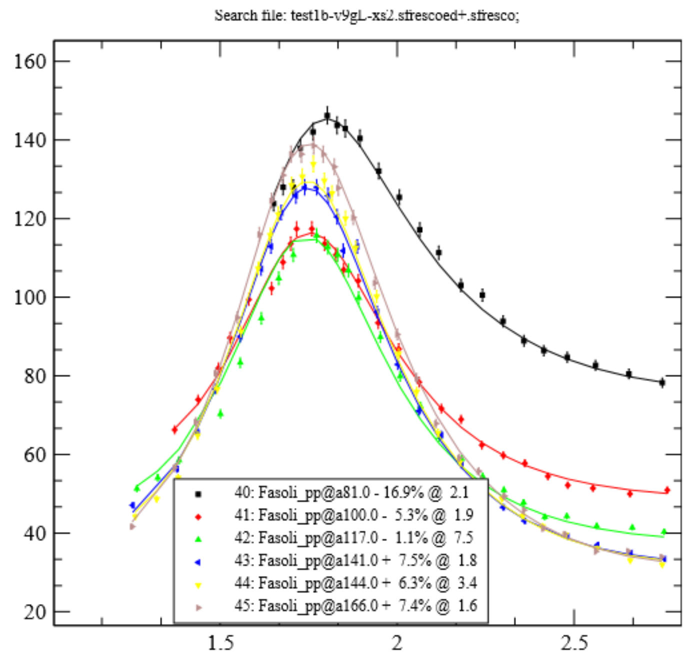
c/o: I. Thompson

R-matrix fit to α-elastic scattering on ^{3}He and proton elastic scattering on ^{6}Li

Dataset	Chisq/pts	av norm
Barnard_aa.dat	0.967	0.990

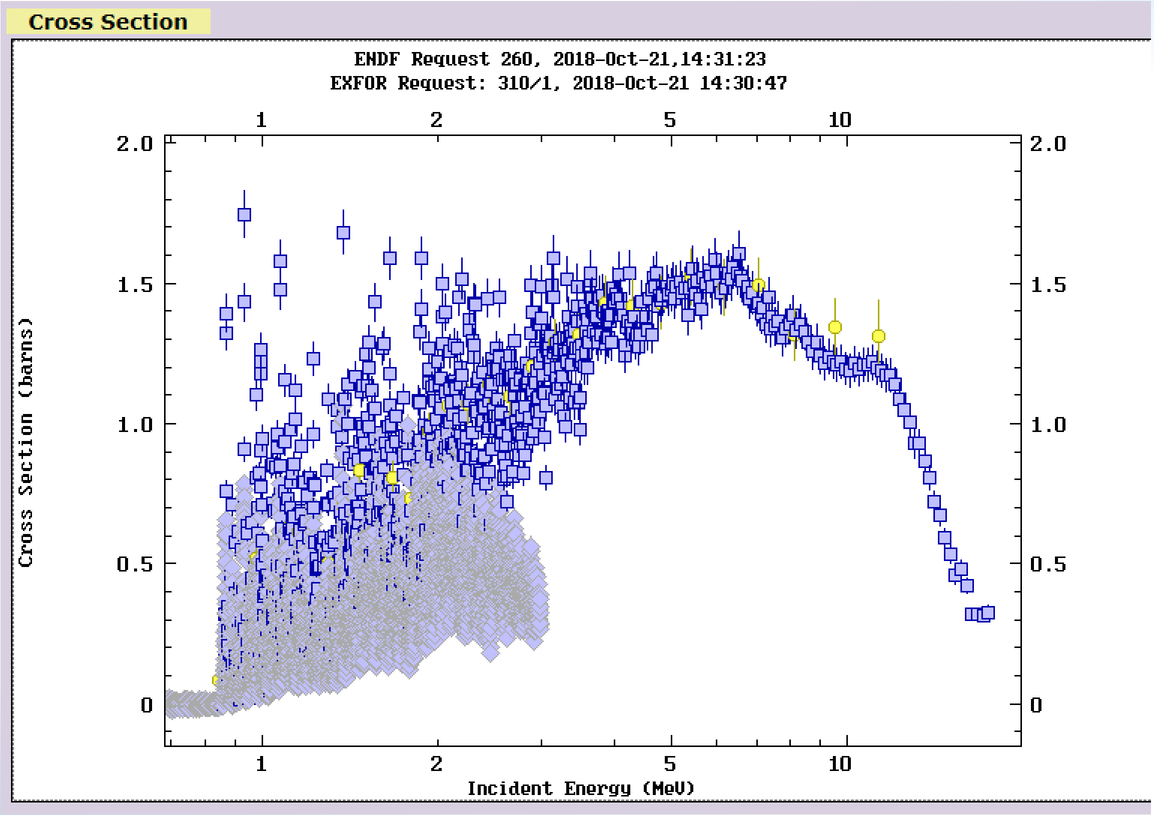


Dataset	Chisq/pts	av norm	av shift
Fasoli_pp.dat	3.895	0.996	

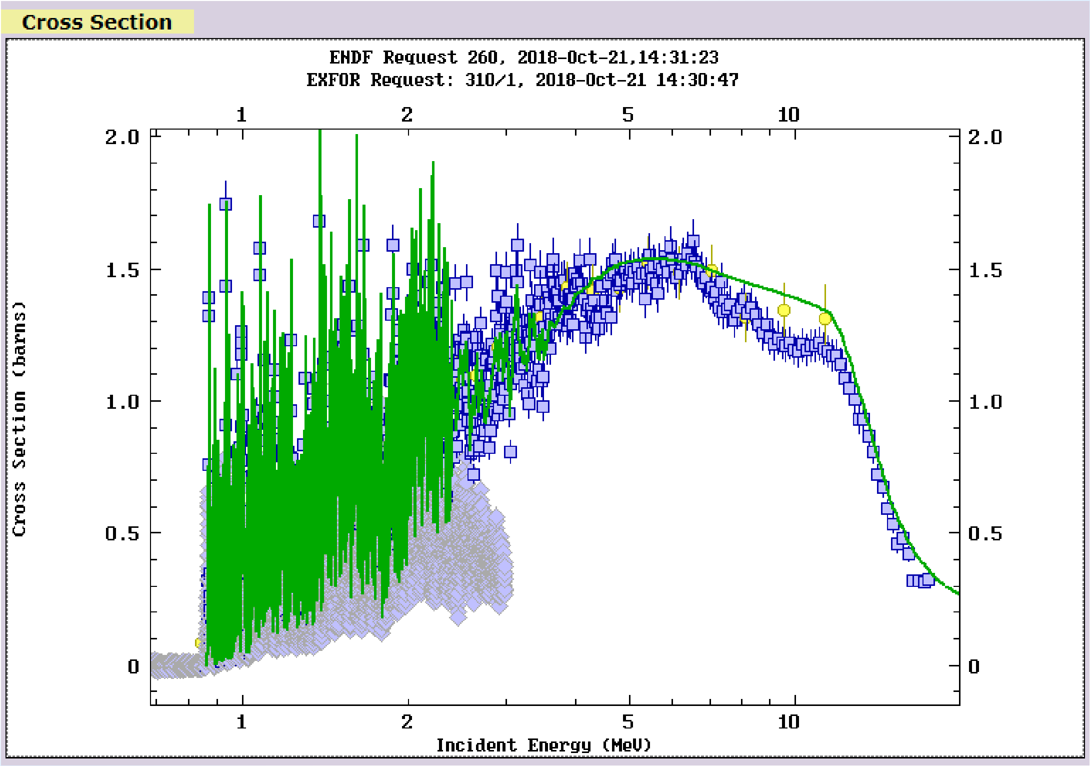


c/o: I. Thompson

Evaluation of nuclear cross sections

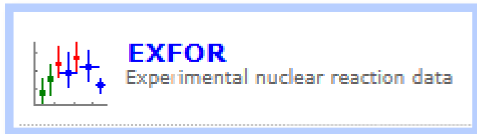


Evaluation of nuclear cross sections

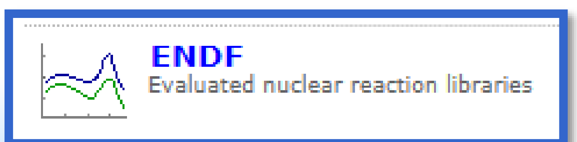


Evaluation methodology

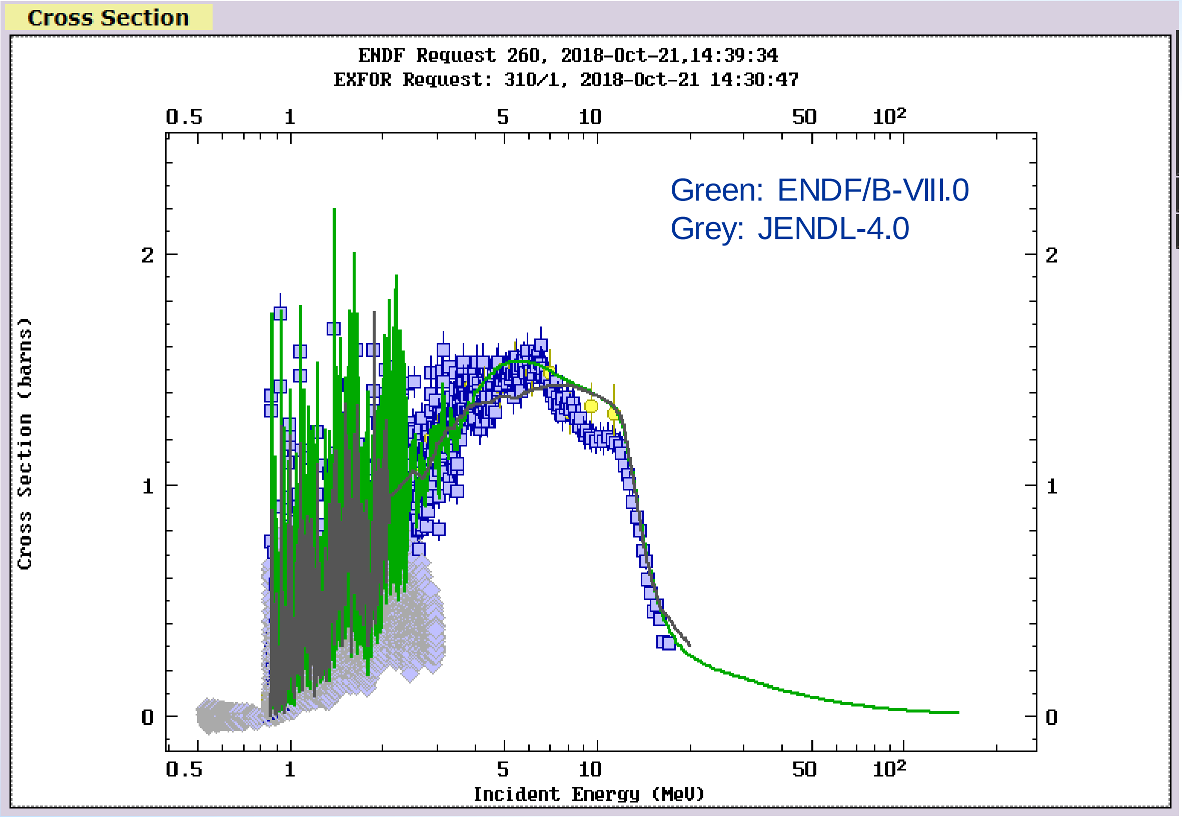
- Compile available exp. data for a specific incident particle on a target nucleus up to energy of interest – include all data in all open reaction channels



- Assess exp. data: identify outliers; adopt final datasets – *subjective*
- Fit cross sections (total, angular distributions, double-differential) in open channels – *subjective*
- Provide recommended cross sections and associated uncertainties (statistical, covariances)



Different evaluations



Types of evaluation

- Based on nuclear models

  model parameter fits to data
  cross-section uncertainties:
  propagation of parameter uncertainties

- Based on cross section space

  initial cross section (prior)
  variation of cross sections to fit the data

- Cubic-spline fit

Types of evaluation

- Based on nuclear models

  model parameter fits to data

  cross-section uncertainties:

  prop

- Based

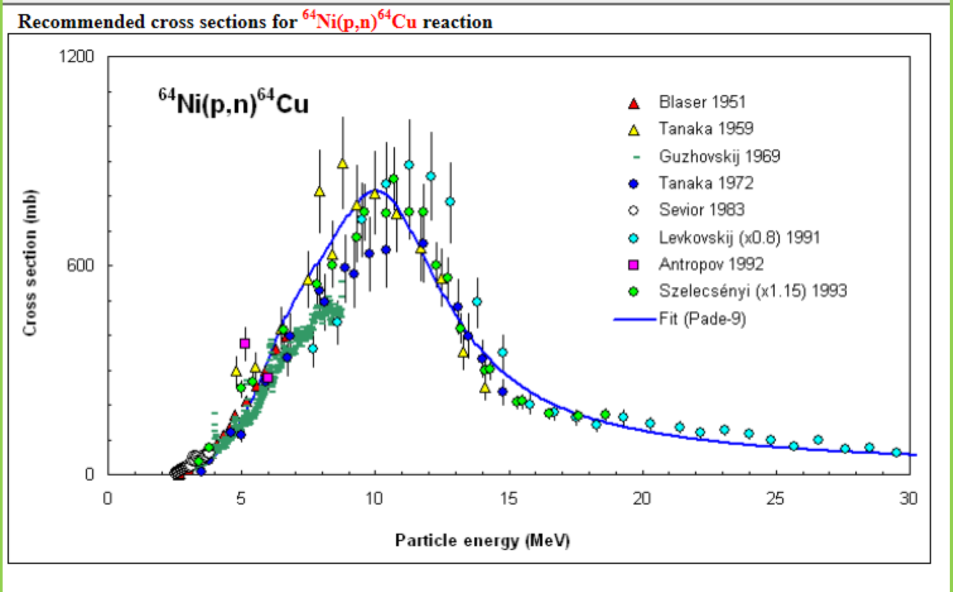
  initia

  MC

  cros

- Cubic-

Example of cubic-spline fit



Uncertainties

mean cross section

\# iterations

spread of the data of cross sections

- Mean: $\mu = \frac{\sum x_i}{N}$
- Variance: $\sigma^2 = \frac{(x_1 - \mu)^2 + \cdots + (x_N - \mu)^2}{N}$
- Standard deviation: $\sigma = \sqrt{\text{variance}} = \sqrt{\sigma^2}$

ex: cross sections at two different energies

- Covariance: $cov(x, y) = \sigma_{xy}^2 = \frac{\sum(x_i - \mu)(y_i - \nu)}{N-1}$

How two variables change together:
Positive (+): move together
Negative (-): move in opposite directions

for $N = 2$: $V_{xy} = \begin{bmatrix} \sigma_x^2 & \sigma_{x,y} \\ \sigma_{y,x} & \sigma_y^2 \end{bmatrix}$

Covariance matrix

- Correlations: $\varrho_{xy} = cov(x, y)/\sigma_x \sigma_y$

measure of the degree to which two variables move together :

-1 to +1: 0 means they are not related

Fitting data: uncertainty propagation

- $\sigma = f(x_1, x_2, \ldots x_N)$
- $\alpha_i = \frac{\vartheta f}{\vartheta x_i} \rightarrow A$
- Mean $\bar{\sigma} = f(\mu, \nu, \ldots)$
- Uncertainty propagation:

$$V_\sigma = A V_x A^T$$

Total σ uncertainty

variance-covariance matrix

Uncertainties

- Multivariate data: $\sigma = f(\overbrace{p_1, p_2, .. p_N}^{\text{ex: energies, angles}})$

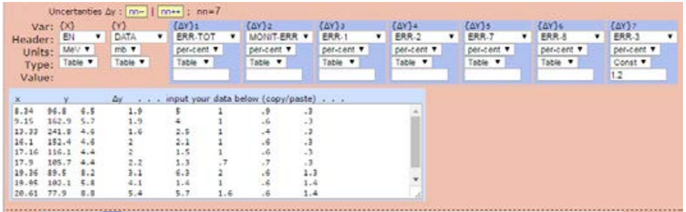
Need to calculate mean vector (mean values) and variance-covariance matrix (diagonal – off diagonal)

Experimental : statistical errors (diagonal) and systematic errors (off diagonal)

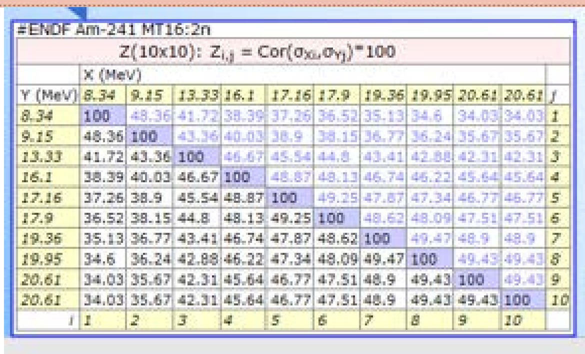
Parameter uncertainties when adjusting model parameters (α_i, α_j, …) to data: $\vartheta^2/\vartheta p_i \theta p_j$

Cross section uncertainties when adjusting cross sections to data: $\mathrm{cov}(\delta\sigma_i, \delta\sigma_j)$

Experimental covariance matrix: EXFOR



input all possible uncertainties statistical & systematic



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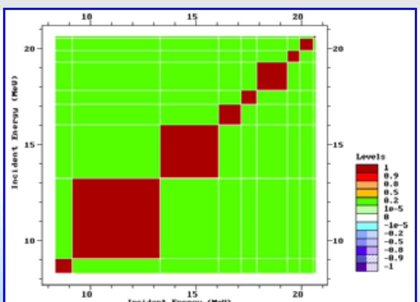
Z(10x10): $Z_{i,j} = \mathrm{Cor}(\sigma_{Xi}, \sigma_{Yj})*100$

	X (MeV)										
Y (MeV)	8.34	9.15	13.33	16.1	17.16	17.9	19.36	19.95	20.61	20.61	j
8.34	100	48.36	41.72	38.39	37.26	36.52	35.13	34.6	34.03	34.03	1
9.15	48.36	100	43.36	40.03	38.9	38.15	36.77	36.24	35.67	35.67	2
13.33	41.72	43.36	100	46.67	45.54	44.8	43.41	42.88	42.31	42.31	3
16.1	38.39	40.03	46.67	100	48.87	48.13	46.74	46.22	45.64	45.64	4
17.16	37.26	38.9	45.54	48.87	100	49.25	47.87	47.34	46.77	46.77	5
17.9	36.52	38.15	44.8	48.13	49.25	100	48.62	48.09	47.51	47.51	6
19.36	35.13	36.77	43.41	46.74	47.87	48.62	100	49.47	48.9	48.9	7
19.95	34.6	36.24	42.88	46.22	47.34	48.09	49.47	100	49.43	49.43	8
20.61	34.03	35.67	42.31	45.64	46.77	47.51	48.9	49.43	100	49.43	9
20.61	34.03	35.67	42.31	45.64	46.77	47.51	48.9	49.43	49.43	100	10
i	1	2	3	4	5	6	7	8	9	10	

estimate correlations among uncertainties i and j (where diagonal i=j means statistical and i≠j means off-diagonal i.e. systematic uncertainties)

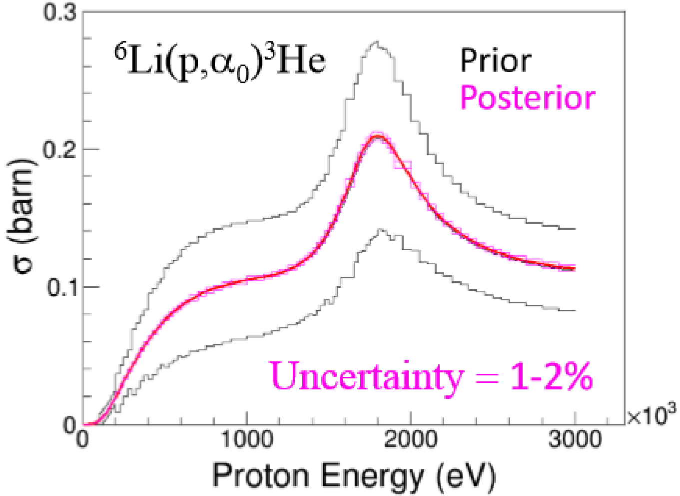


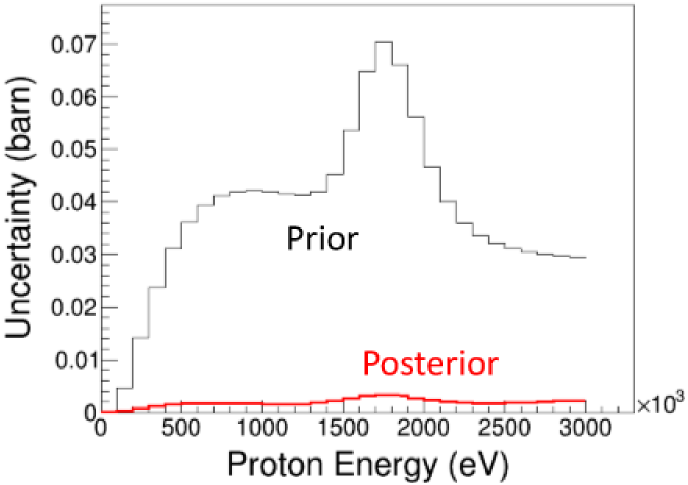
from correlation matrix calculate covariance

See V. Zerkin's lecture

Example: R-matrix fit

Uncertainty for $^{6}Li(p,\alpha)^{3}He$

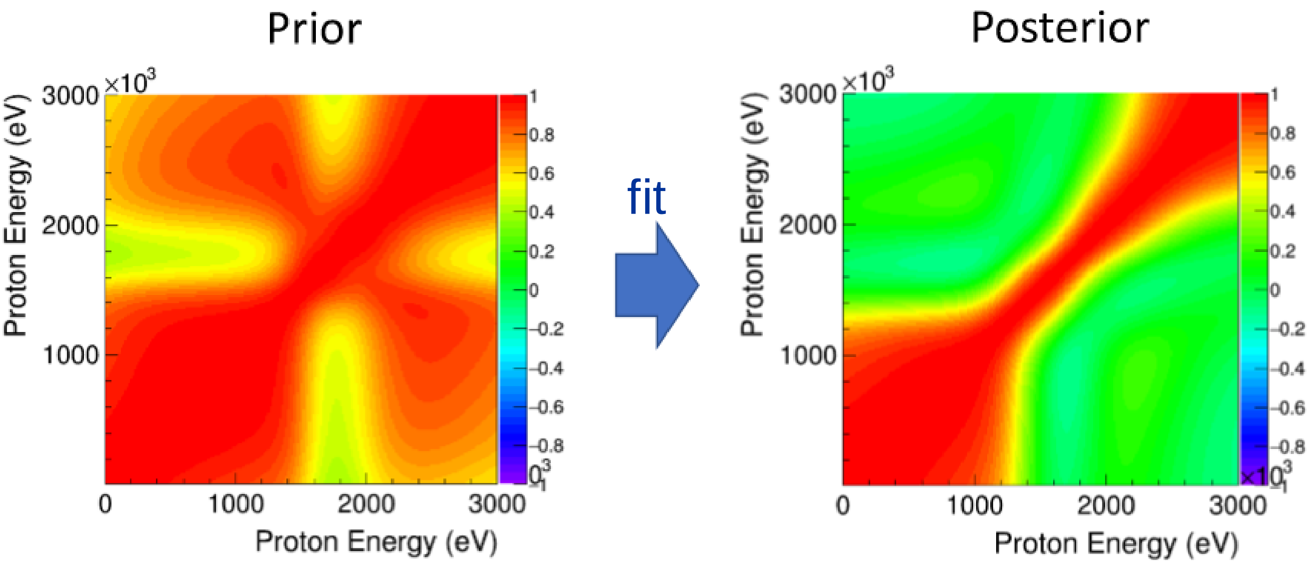




c/o: S. Kunieda

Example cont'd

Correlation matrix for ${}^{6}\mathrm{Li}(p,\alpha){}^{3}\mathrm{He}$

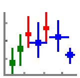


- Off-diagonal correlations are reduced
- Strong correlations at lower and higher energies

c/o: S. Kunieda

To summarize:

Compilation



EXFOR
Experimental nuclear reaction data

Archival

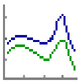
Evaluation

Model/cross section fits
Least Squares/Bayesian inference
Cross sections & Covariances

Verification/ Validation

Benchmark differential cross sections against integral measurements

Dissemination



ENDF
Evaluated nuclear reaction libraries

ENDF/B-VIII, JEFF, JENDL

IAEA
International Atomic Energy Agency
Atoms for Peace and Development

Thank you!