The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2141-23

Joint ICTP-IAEA Workshop on Nuclear Reaction Data for Advanced Reactor Technologies

3 - 14 May 2010

Cross Section Measurements and Uncertainties of Cross Section Data

PLOMPEN A.

EC-JRC_IRMM
Geel
BELGIUM

Joint Research Centre (JRC)

Cross section measurements and uncertainties of cross section data

Arjan Plompen

European Commission, Joint Research Centre,

Institute for Reference Materials and Measurements

http://www.jrc.ec.europa.eu/

Overview

General introduction

Some detailed measurement examples

Uncertainties in measurement

Summary part 1

Data of interest
Use of uncertainties
Need for measurements

Cross section
total, fission, elastic
inelastic, residual or
ejectile yields

Differential cross section

- Angular distribution
- Emission spectrum
- Double differential

Other parameters

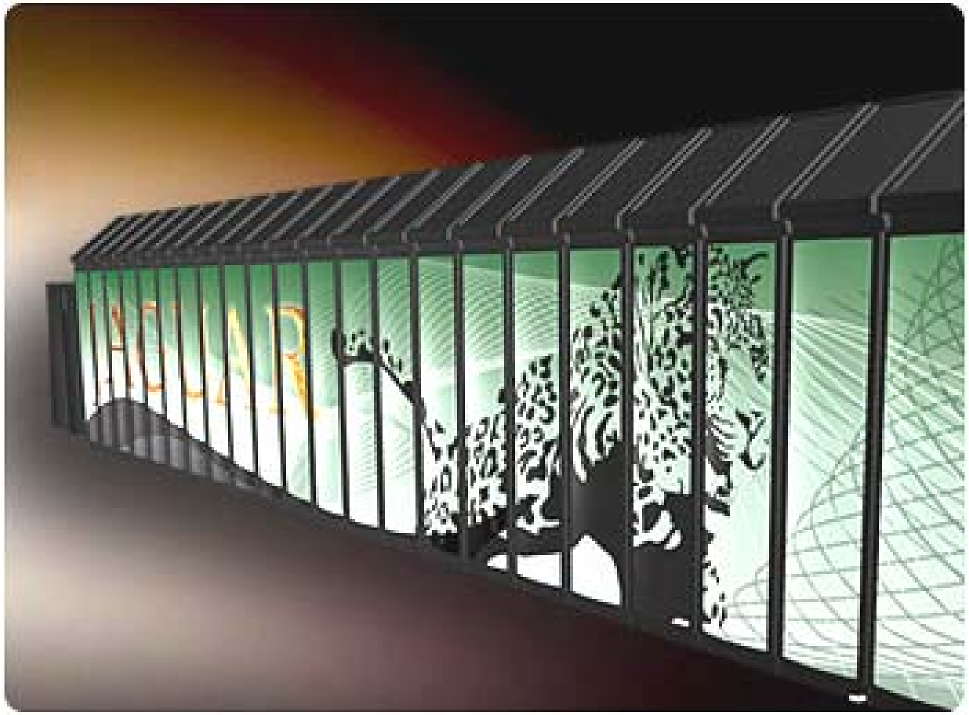
Resonance parameters

Influence quantities
Doppler broadening
Instrumental broadening
Sample broadening
Temperature
Pressure
Sample composition, impurities, dimensions, roughness,…
Room return
Collimation
Neutron sources

Why cross sections, … (nuclear) data ?

Computing power, data storage and manipulation, modeling improvements are increasingly determining the landscape of science

The possibilities are still poorly explored but new developments continuously push frontiers

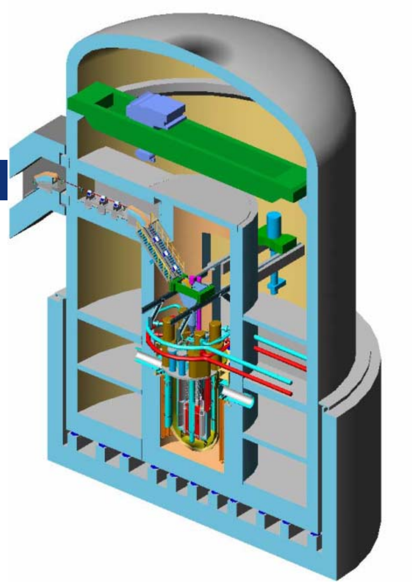


Oak Ridge National Laboratory's Cray XT5 "Jaguar" Supercomputer Current #1 supercomputer

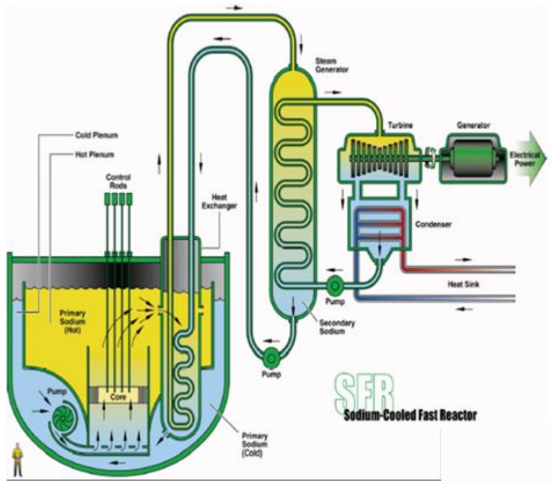
2 petaflops peak

... to address some of the most challenging scientific problems in areas such as climate modeling, renewable energy, materials science, fusion and combustion...
.... Novel Computational Impact on Theory and Experiment (INCITE) program....

Why cross sections, … (nuclear) data ?



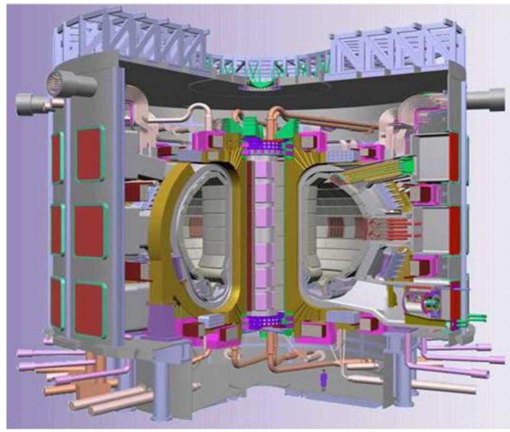
Modeling of reactors



Two important equations

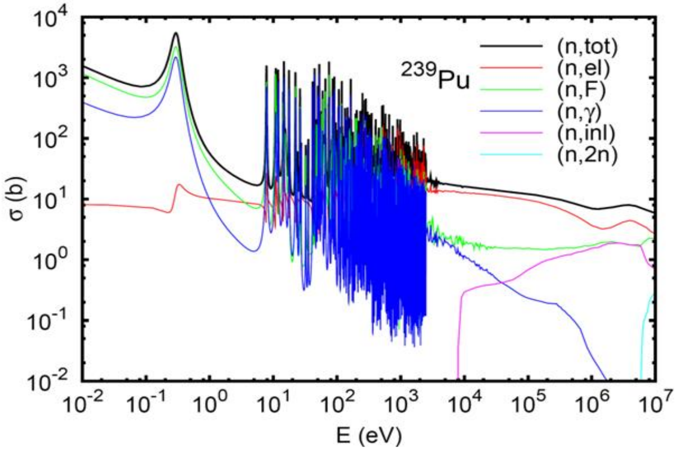
Neutron transport: Boltzmann

Nuclides inventories: Bateman



… and charged particles, photons, ….
(Encoded in discrete ordinates or Monte Carlo codes)

Equations, models, computing power are not enough!
Constants of nature are required!



Boltzmann equation, quantities and required data

$$\frac{1}{v}\frac{\partial f}{\partial t} + \boldsymbol{\Omega}\cdot\nabla f + \Sigma_T f = S + \int dE' d\boldsymbol{\Omega}' \, f(E',\boldsymbol{\Omega}')\Sigma_S(E'\to E, \boldsymbol{\Omega}'\to\boldsymbol{\Omega})$$

$$S = S_{PF} + S_{dn} + S_{\alpha n} + S_{\text{ext}}$$

$$S_{PF} = \sum_i N_i \int dE' \, f(E')\overline{\nu}_i(E')\sigma_{F,i}(E') f_{P,i}(E',E)$$

$$\Sigma_{S}(E\to E',\boldsymbol{\Omega}\to\boldsymbol{\Omega}') = \sum_i N_i \frac{d^2\sigma_{s,i}}{dE'd\Omega'}(E,E',\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}')$$

$$\Sigma_T = \sum_i N_i \sigma_{T,i}$$

Doppler ignored

$$\Sigma_T = \Sigma_a + \Sigma_s$$

$$\Sigma_s = \int dE' d\boldsymbol{\Omega}' \, \Sigma_S(E\to E',\boldsymbol{\Omega}\to\boldsymbol{\Omega}')$$

Bateman equation, quantities and required data

$$\frac{dN_i}{dt} = -\lambda_i N_i - r_i N_i + \sum_{j \neq i} \left\{ \lambda_{j \to i} + r_{j \to i} \right\} N_j$$

N_i / N_j =concentration of nuclide i/j

λ_i $= \frac{\ln 2}{T_{1/2,i}} = \sum_{j \neq i} \lambda_{i \to j}$ = the decay constant of nuclide i

$\lambda_{i \to j}$ $= \lambda_i b_{i \to j}$

$b_{i \to j}$ =probability for decay of isotope i to j

r_i $= \int dE\, \Phi(E,t) \sigma_{a,i}(E) = \sum_{j \neq i} r_{i \to j}$

$\sigma_{a,i}$ =absorption(=removal) cross section for isotope i

$r_{i \to j}$ $= \int dE\, \Phi(E,t) \sigma_{a,i \to j}(E)$

$\sigma_{a,i \to j}$ =cross section for transforming isotope i to j

This talk: Nuclear Data

Thermo-hydraulic

- Heat transport
- Coolant flow
- …

Chemical

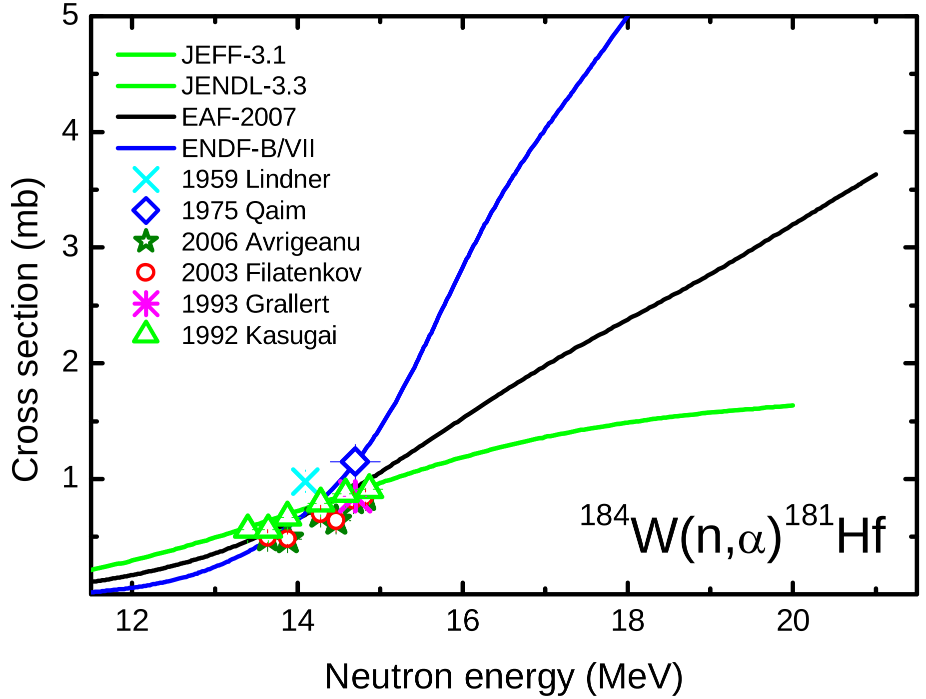
- Fuel fabrication
- Reprocessing
- Partitioning
- Conditioning
- Corrosion
- …

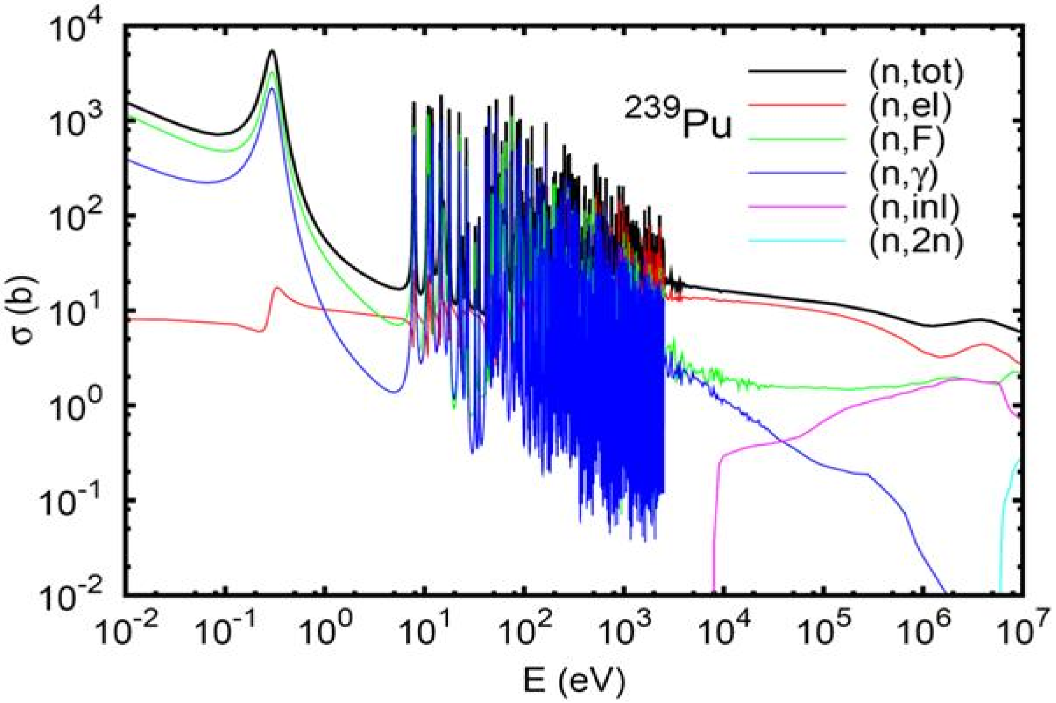
But there are others…
… for other processes
… involving other equations
… increasingly integrated approaches are seen (microscopic-macroscopic approach, global modeling)

Mechanical

- Densities, …
- Strength/stress, …
- Radiation damage
- …

Why cross section/reaction parameter measurements?



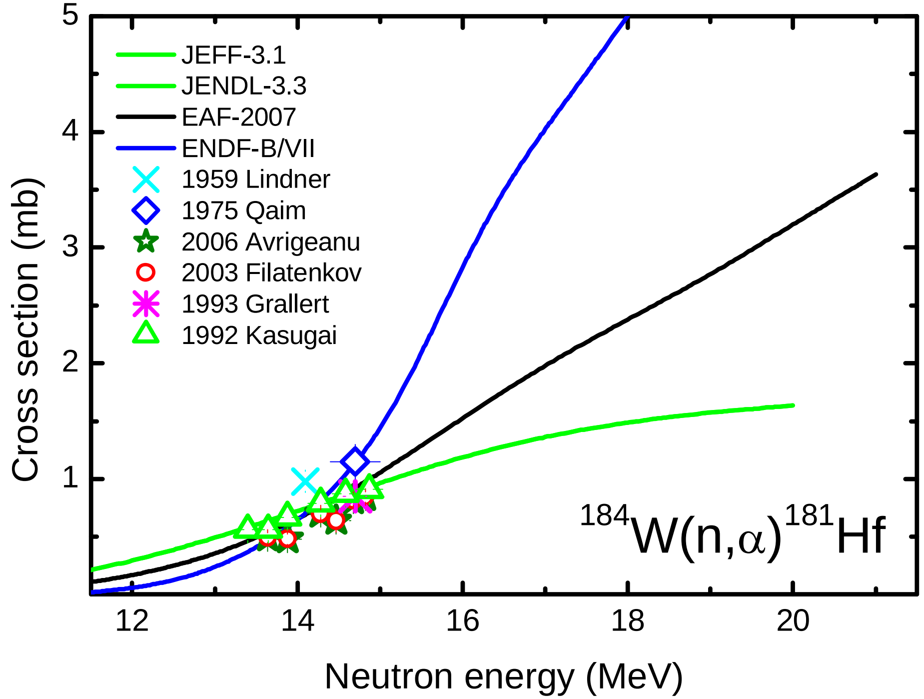


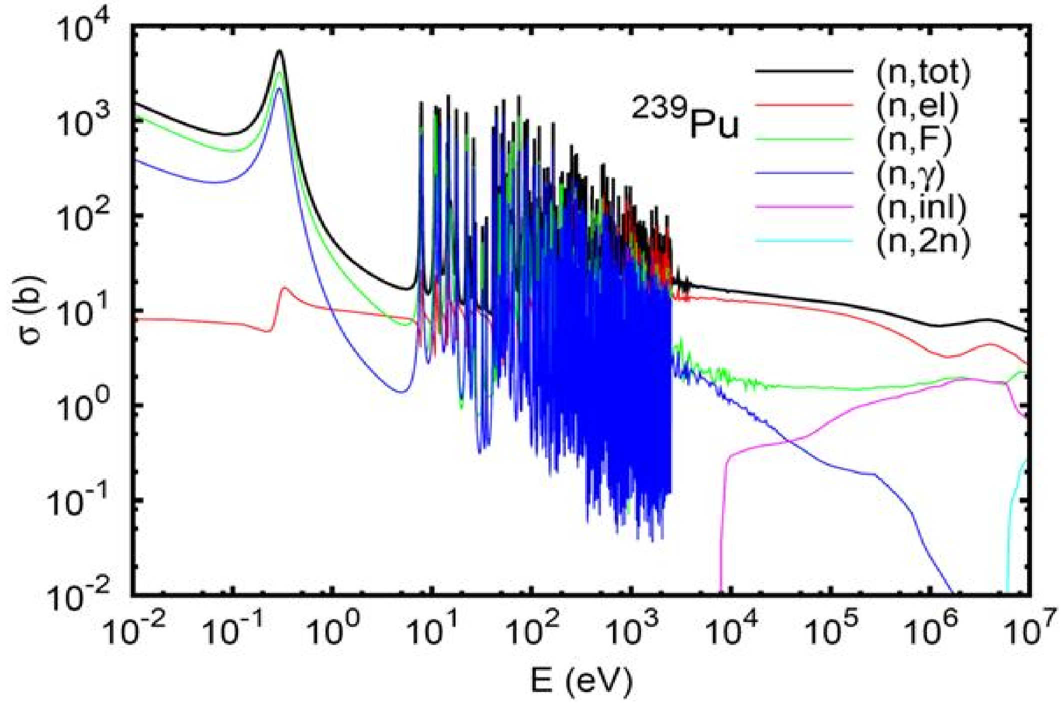
Nuclear modeling lacks accuracy for detailed predictions of cross sections

Resonance parameters are effectively stochastic variables
level energies, partial widths

Data are needed for developing models, determining model parameters, benchmark model parameter databases and overall model performance

Why cross section/reaction parameter measurements?

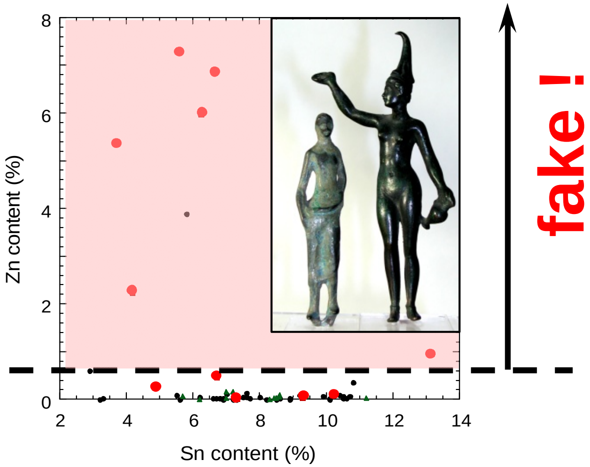


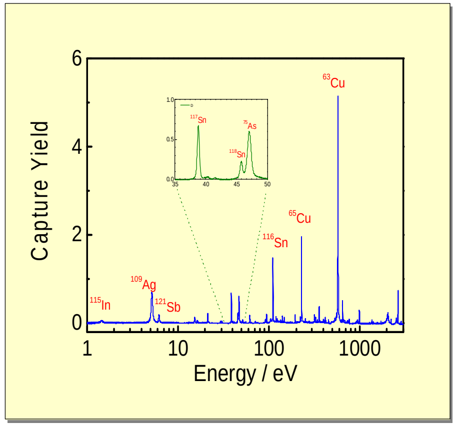


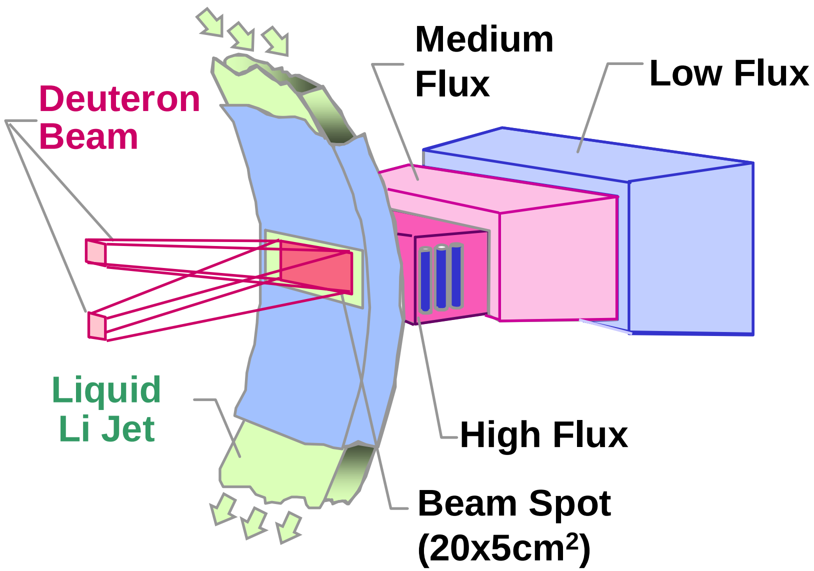
On the other hand:
Modeling is essential to

- ☑ **extract the physical parameters from a measurement**
- ☑ **interpolate and extrapolate from experimental results**
- ☑ **make an educated guess about the unmeasurable**
- ☑ **provide complete physically consistent databases**

Other motivations than NPP…







Important challenges:

Plant life time

Fuel economy

Waste minimization

- Transmutation
- **Elimination** of all actinides (99.5-99.9%)
- Th/U fuel cycle

Sustainability of (nuclear) energy

- Utilization of resources, global warming, …
- Fast reactors
- …**recycling**…
- Higher burnup, Th/U, …

Subgroup 26 (SG26), M. Salvatores, coordinator (CEA/FZK/ANL)

Subgroup 26 is a working group of the Nuclear Energy Agency's Working Party on Evaluation Cooperation

It addressed the nuclear data needs likely to arise from design/optimization requirements in fast reactor development

General philosophy

- ☑ Choose the target systems (GenIV, GNEP, references)
- ☑ Choose key system parameters
- ☑ Fix their target accuracies
- ☑ Perform a sensitivity analysis
- ☑ Determine corresponding data uncertainties

⇨ **Nuclear data needs**
nuclide, process, energy range

http://www.nea.fr/dbdata/html

System modeling

A simple principle
Conceptual systems
Good understanding

Future

- Better capabilities
- More modeling
- More systematic

Q: system parameters
p: nuclear data
f: the model

$$\mathbf{Q} = \mathbf{f}(p)$$

$\mathbf{Q} = (Q_1, Q_2, ..., Q_k)$ = the list of system quantities

$\mathbf{p} = (p_1, p_2, ..., p_n)$ = the list of model parameters

$\mathbf{f} = (f_1, f_2, ..., f_k)$ = the model description

$\mathbf{p}$ tuned so that $\mathbf{Q}$ as desired

$\mathbf{p}$ includes all cross sections for all isotopes

e.g. Q_1= the SFR BOL multiplication factor

e.g. Q_{200}=the EOL amount of ^{241}Am in a PWR,...

e.g. p_{100}=fission cross section ^{239}Pu in group 12

e.g. p_{200}=fractional yield of ^{242g}Am in $^{241}Am(n,\gamma)$,...

$$V_{ij}(\mathbf{Q}) \equiv \langle \delta Q_i \delta Q_j \rangle = \sum_{a,b} \frac{\partial f_i}{\partial p_a} \frac{\partial f_j}{\partial p_b} \langle \delta p_a \delta p_b \rangle$$

Relative covariance

$$R_{ij}(\mathbf{Q}) \equiv \frac{V_{ij}(\mathbf{Q})}{Q_i Q_j} = \sum_{a,b} S_{ia} S_{jb} R_{ab}(\mathbf{p})$$

Sensitivity coefficient: $S_{ia} \equiv \frac{p_a}{f_i} \frac{\partial f_i}{\partial p_a}$

$$R_{ij}(\mathbf{Q}) = \sum_{a,b} S_{ia} S_{jb} C_{ab}(\mathbf{p}) r_a(\mathbf{p}) r_b(\mathbf{p})$$

$$C_{ab}(\mathbf{p}) \equiv \frac{V_{ab}(\mathbf{p})}{u_a(\mathbf{p}) u_b(\mathbf{p})} \implies R_{ab} = C_{ab} r_a r_b$$

Uncertainty analysis
System versus data:
Uncertainty propagation
Sensitivity analysis

V (co)variance matrix
S sensitivity matrix
R relative cov. matrix
C correlation matrix

Uncertainty $u_a(\mathbf{p}) \equiv \sqrt{\langle \delta p_a \delta p_a \rangle}$

Relative uncertainty $r_a(\mathbf{p}) \equiv \frac{u_a(\mathbf{p})}{p_a}$

Correlation matrix ($C_{aa} = 1$)

Back propagation method

System uncertainty limits L_i:

$$r_i(\mathbf{Q}) < L_i \quad \text{for } 1 \leq i \leq k$$

Equivalently for the parameters:

$$\sum_{a,b} S_{ia} S_{ib} C_{ab}(\mathbf{p}) r_a(\mathbf{p}) r_b(\mathbf{p}) < L_i^2, \quad i = 1..k$$

For each Q_i an ellipsoid in $\mathbf{r}(\mathbf{p})$-space

$$\min\left(\sum_a \frac{\lambda_a}{r_a^2(\mathbf{p})}\right)$$

The cost parameters λ_a may be changed according to the relative difficulty of obtaining low uncertainties for the parameter p_a.

L: System parameter constraints

Ellipsoids in relative uncertainty space of the data

One ellipsoid per system parameter

…. Still leave a domain of acceptable uncertainties

Use freedom to find best route to final goal:

Cost function to weigh relative difficulty for improvement of the data.

SG26 example shows

Use of data in reactor modeling

Use of uncertainties in reactor modeling

Role of data uncertainties

Role of uncertainty correlations

The benefits of sensitivity analysis to identify important issues in nuclear data (or other data/effect studies)

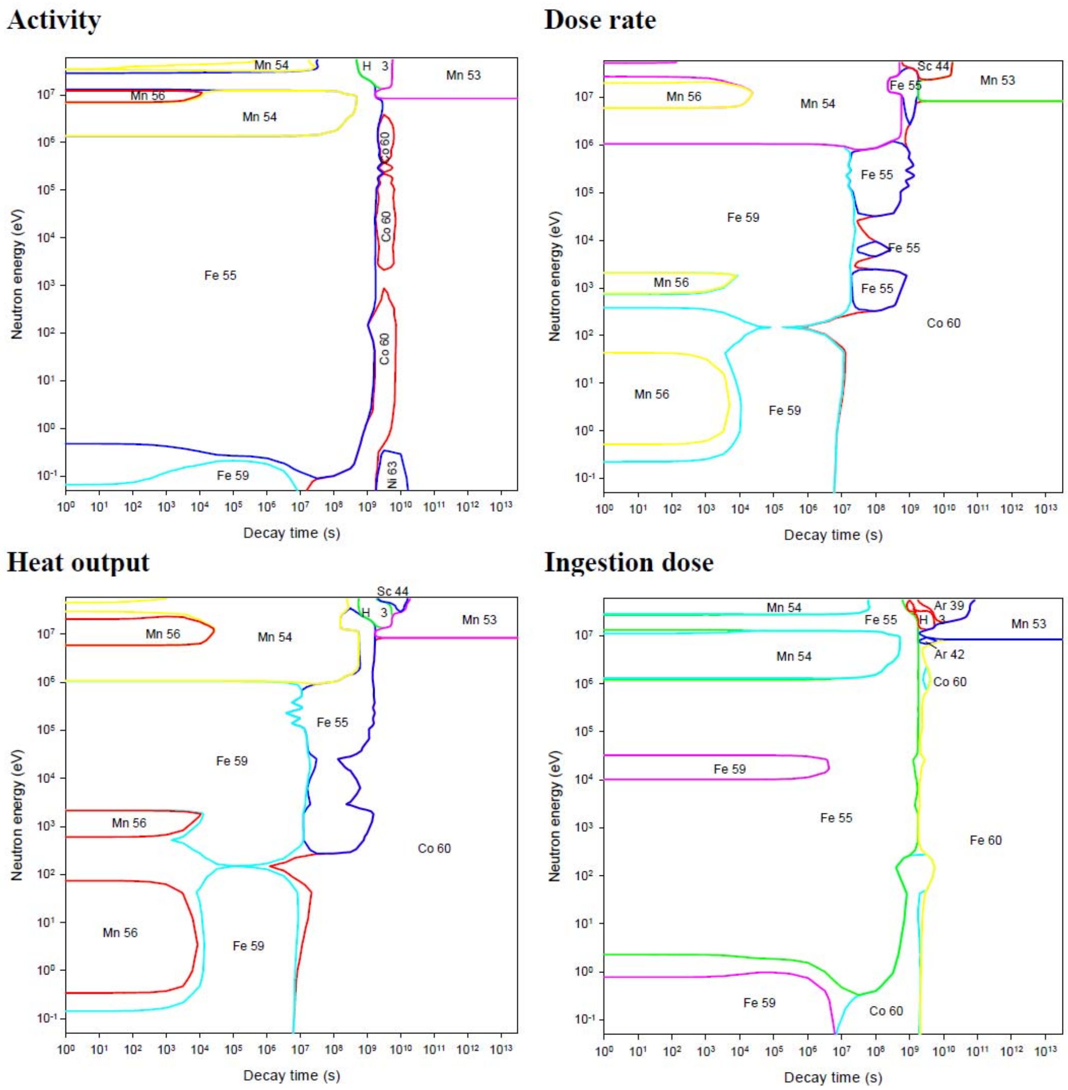
Other ways of identifying needs

Importance Diagrams

Activation data

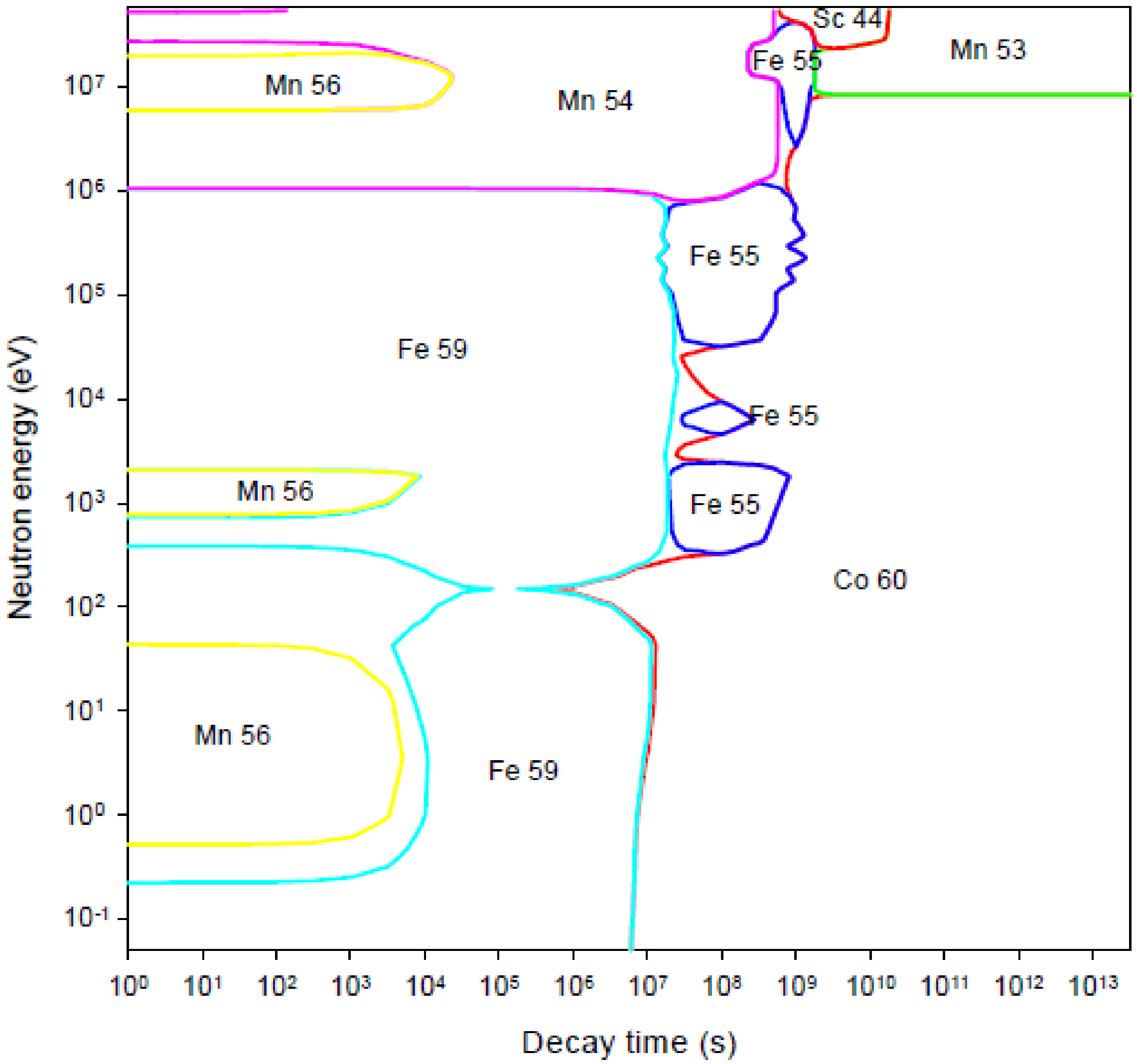
UKAEA report 552 Handbook of Activation data calculated using EASY-2007 (2009)

Iron importance diagrams & transmutation



Other ways of identifying needs

Dose rate



Nuclear data needs

Established network and procedures

- Feedback from users and validation
- New measurement and evaluation
- Quality cycle

International fora (WPEC, JEFF, OECD-NEA, IAEA)

Collaborations (DOE, BNL, JAEA, Russia, Korea, China, India,….)

High priority request list for nuclear data (OECD-NEA)

www.nea.fr/html/dbdata/hprl

Reaction data

Main topic

Decay data

Some comments only

Measurements of nuclear data

Decay data

Half life

Type: γ, CE, β^-, β^+, ε, n, α, SF

Emission energies, spectra, probabilities

Residual nuclide level and decay scheme

Measurements

Nuclear structure studies

Gammasphere, Euroball, Eurogam, Exogam, Miniball …Agata, Greta
Large specialized community

Radionuclide metrology

Accurate data for calibration sources
Accurate sources (α,β,γ,F)
Methods of measurement

Reaction data

Large field, many aspects

Projectile + target
- Projectile: γ, e, n, p, d, α
- Target: nucleus (Z, A)

Transport and energy loss
- Elastic scattering
- Inelastic scattering

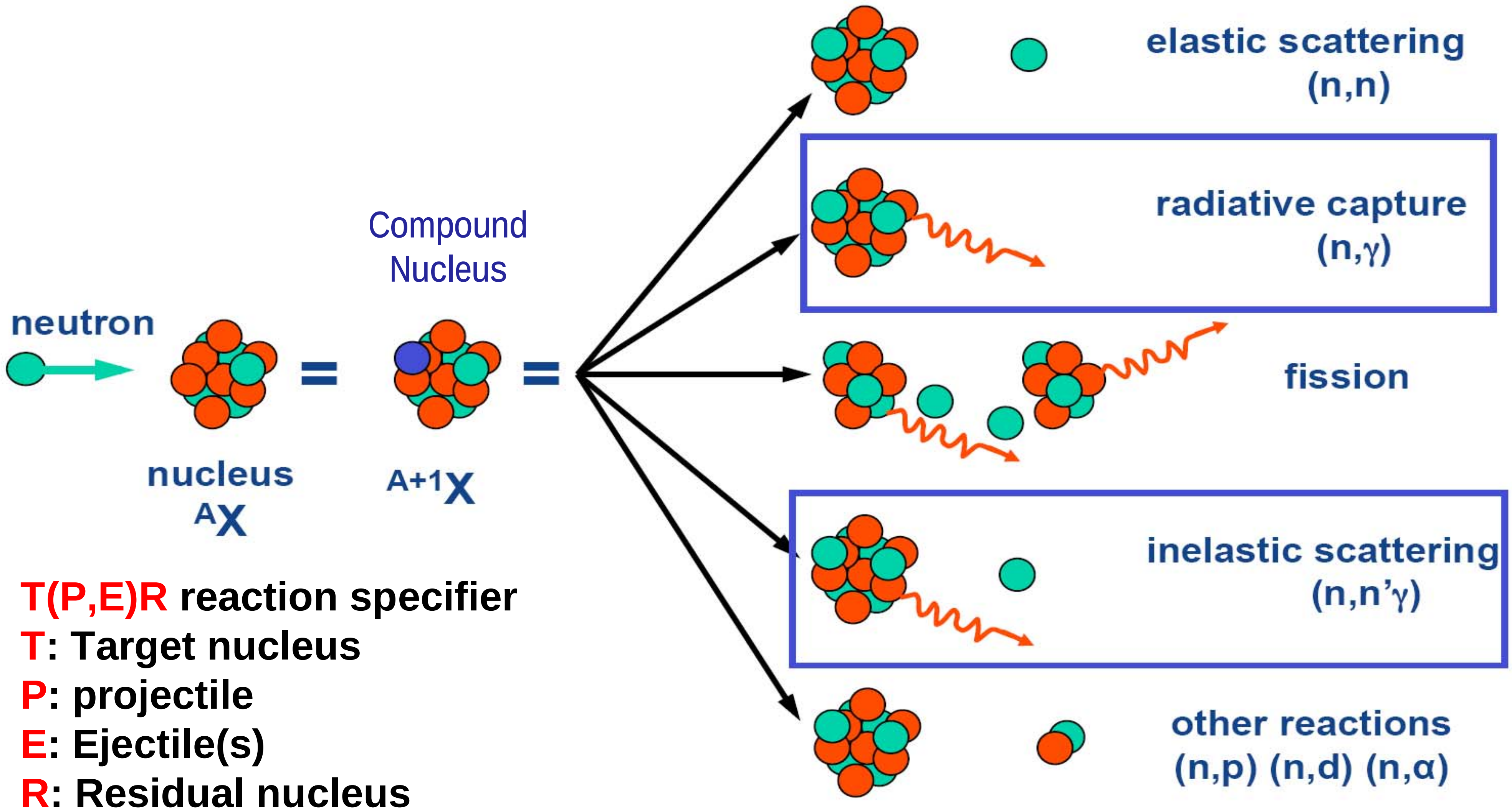
'Real' reactions
- Capture
- Light particle emission
- Fission
- Spallation

Main interest:

Neutrons as projectile
- Energy release
- Neutron production
- Neutron removal
- Neutron energy loss
- Neutron transport
- Production of residuals
- Activation products

Gammas, protons, alphas as projectile
- Heating
- Neutron production
  - Residual neutron source
  - Subcritical assemblies
  - Experimental facilities

Neutron-induced reactions

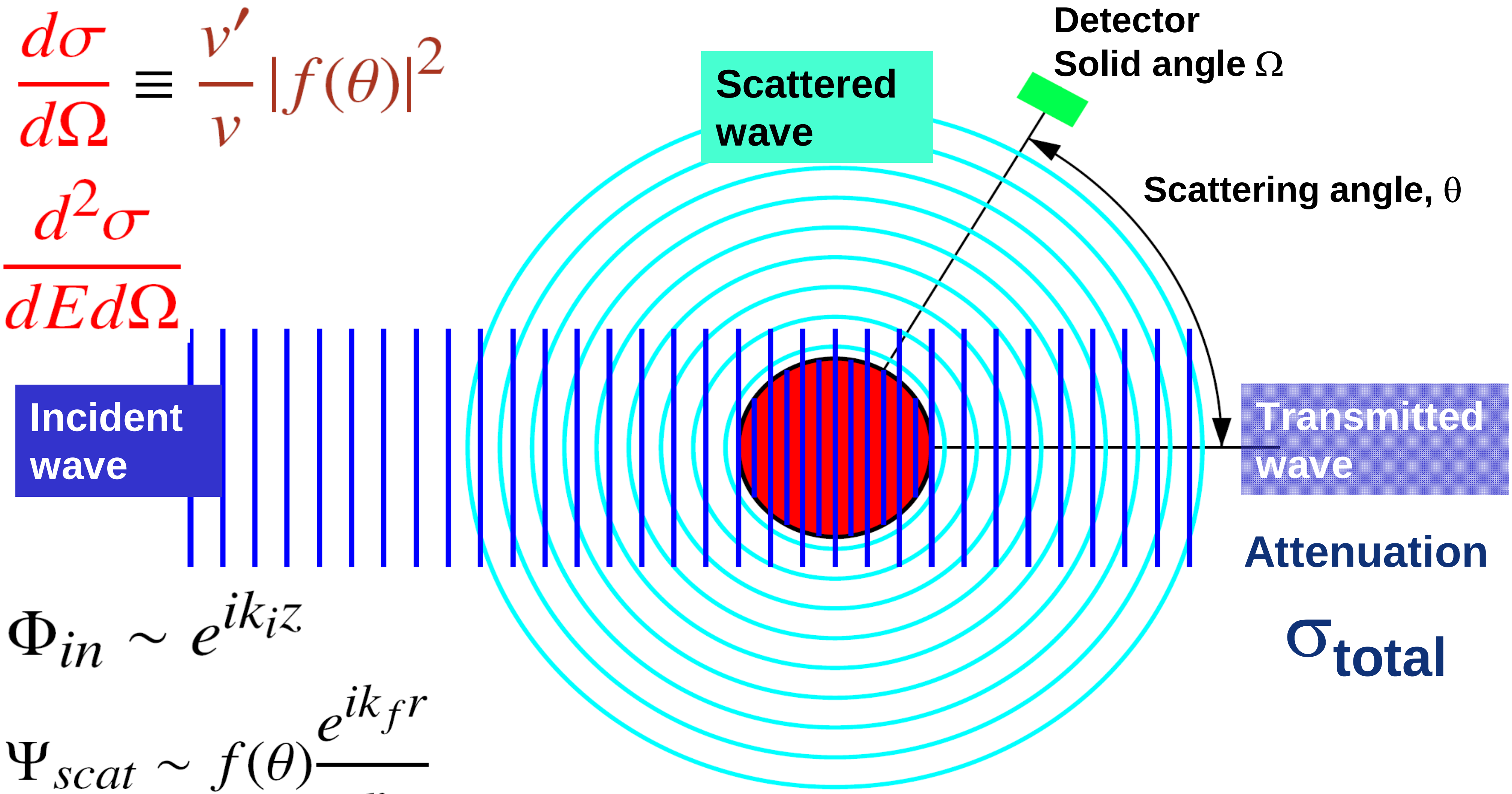


T(P,E)R reaction specifier
T: Target nucleus
P: projectile
E: Ejectile(s)
R: Residual nucleus

Reaction rates: cross section

$$\frac{d\sigma}{d\Omega} \equiv \frac{v'}{v}|f(\theta)|^2$$

$$\frac{d^2\sigma}{dE\,d\Omega}$$



$$\Phi_{in} \sim e^{ik_i z}$$

$$\Psi_{scat} \sim f(\theta)\frac{e^{ik_f r}}{r}$$

Definition and measurements of cross section

$$\sigma \equiv \frac{\text{Reaction rate}}{\text{flux}}(\text{per target nucleus}) = \frac{\dot{R}}{\Phi}$$

$$\sigma = \frac{\text{\# reactions}}{\text{fluence}}(\text{per target nucleus}) = \frac{R}{\mathbf{F}}$$

$$\mathbf{F} = \Phi t, \mathbf{R} = \dot{\mathbf{R}} t, t = \text{measurement time}$$

Rate must be specified

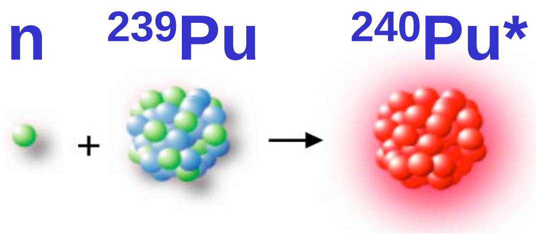
Process (fission, elastic, etc)
energy of particle(s) (E, E')
angle of particle(s) (θ, dΩ')
Number of particles,
Etc.

Measurements

Rate of process
Fluence/normalization
Number of target nuclides

Influence parameters

The resonance range, resolvable and unresolvable structures



Excitation: n+^{239}Pu

J^{π} = 0^+ & 1^+ (s-waves, low E_n)

$\Gamma \approx$ 50 meV

$\tau \approx 1.3\ 10^{-14}$ s

Typical $E_x = S_n + E_0$

Sn = 6.53420 10^6 eV

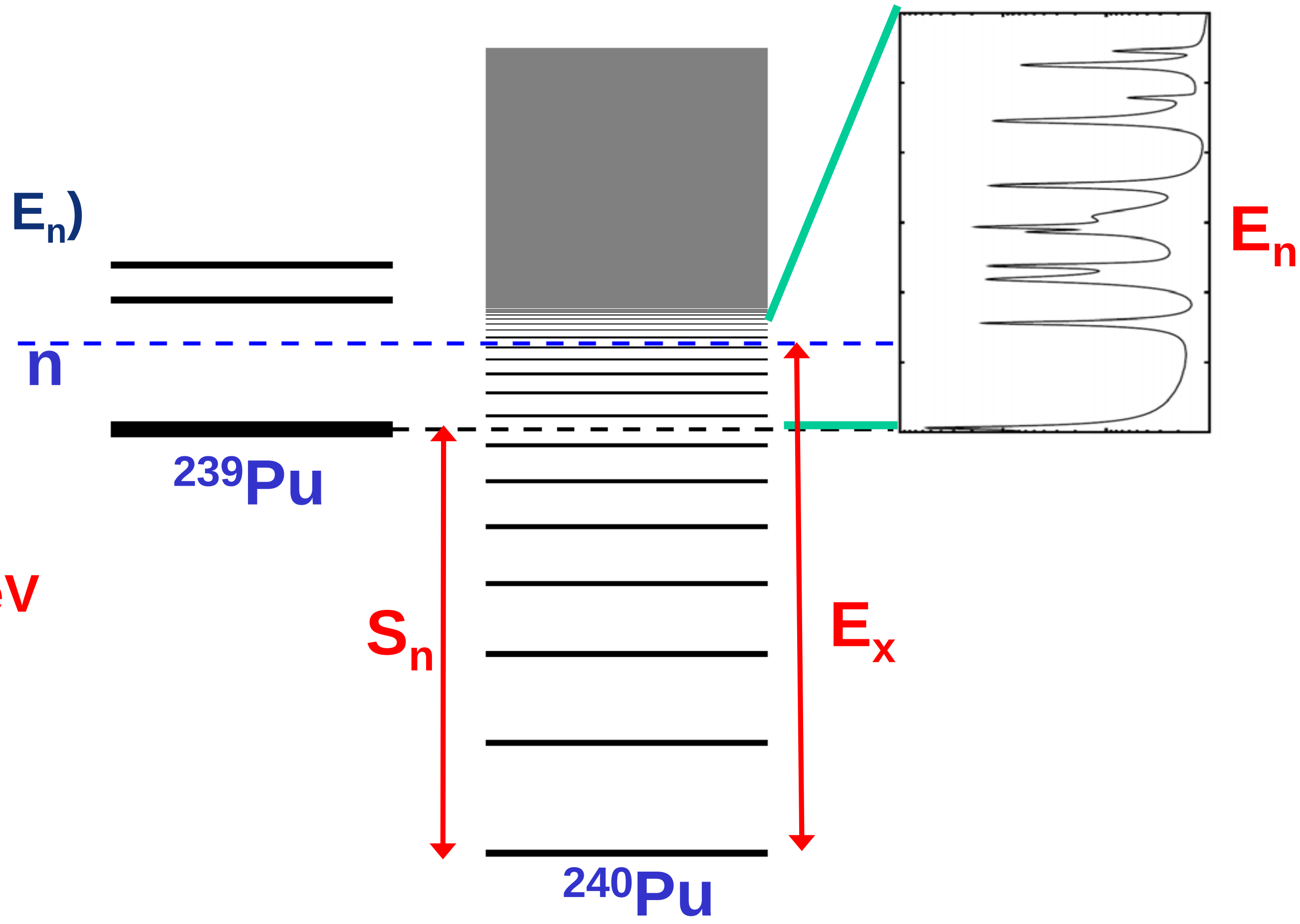
$E_0 \geq 0.2956$ eV

Typical spacing D_0=2.07 eV

$$D \sim E^{5/4} e^{-2\sqrt{aE}}$$

$$a \approx 23.55\ \text{MeV}^{-1}$$

Overlap at $E_x \approx$ 2.3 MeV



The resolved resonance range: resonance parameters

Excitation and decay of an intermediate metastable state
Channels, i=initial, f=final

Excitation: $P_e = \Gamma_i / \Gamma$

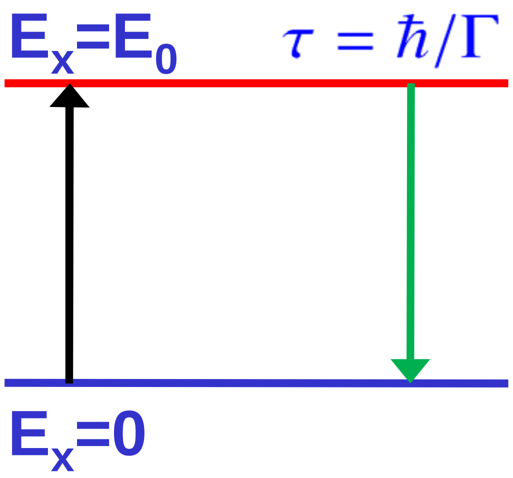
Decay: $P_d = \Gamma_f / \Gamma$

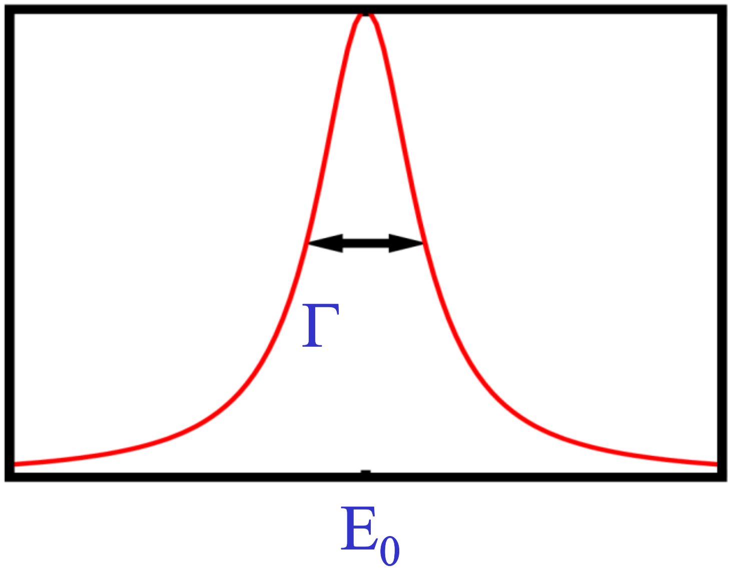
$$\sigma_a(E) = \frac{\pi}{k^2} g_J \frac{\Gamma_i \Gamma_f}{(E - E_0)^2 + \Gamma^2/4}$$

$$\Gamma = \sum_f \Gamma_f$$

Mean life time τ

Natural line width Γ





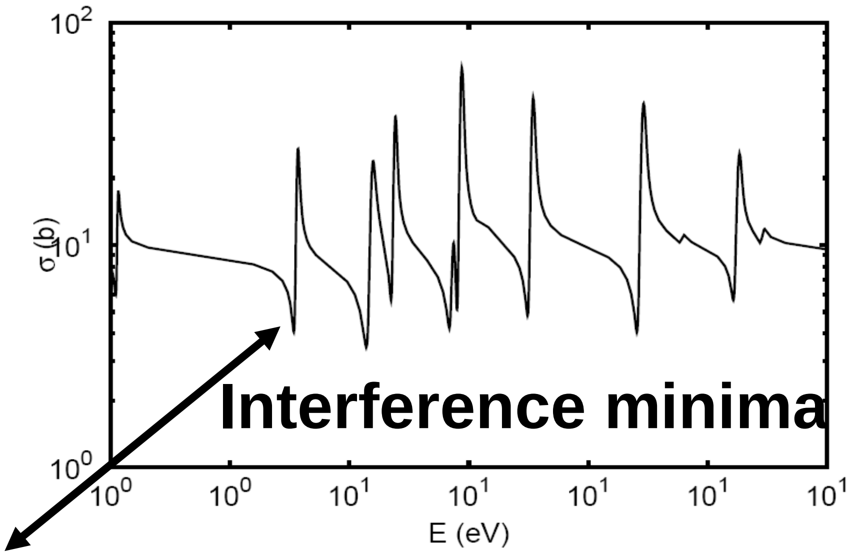
Measurements of nuclear reaction data

$$\sigma_a(E) = \frac{\pi}{k^2} g_J \frac{\Gamma_i \Gamma_f}{(E - E_0)^2 + \Gamma^2/4}$$

Spin factor

in

out



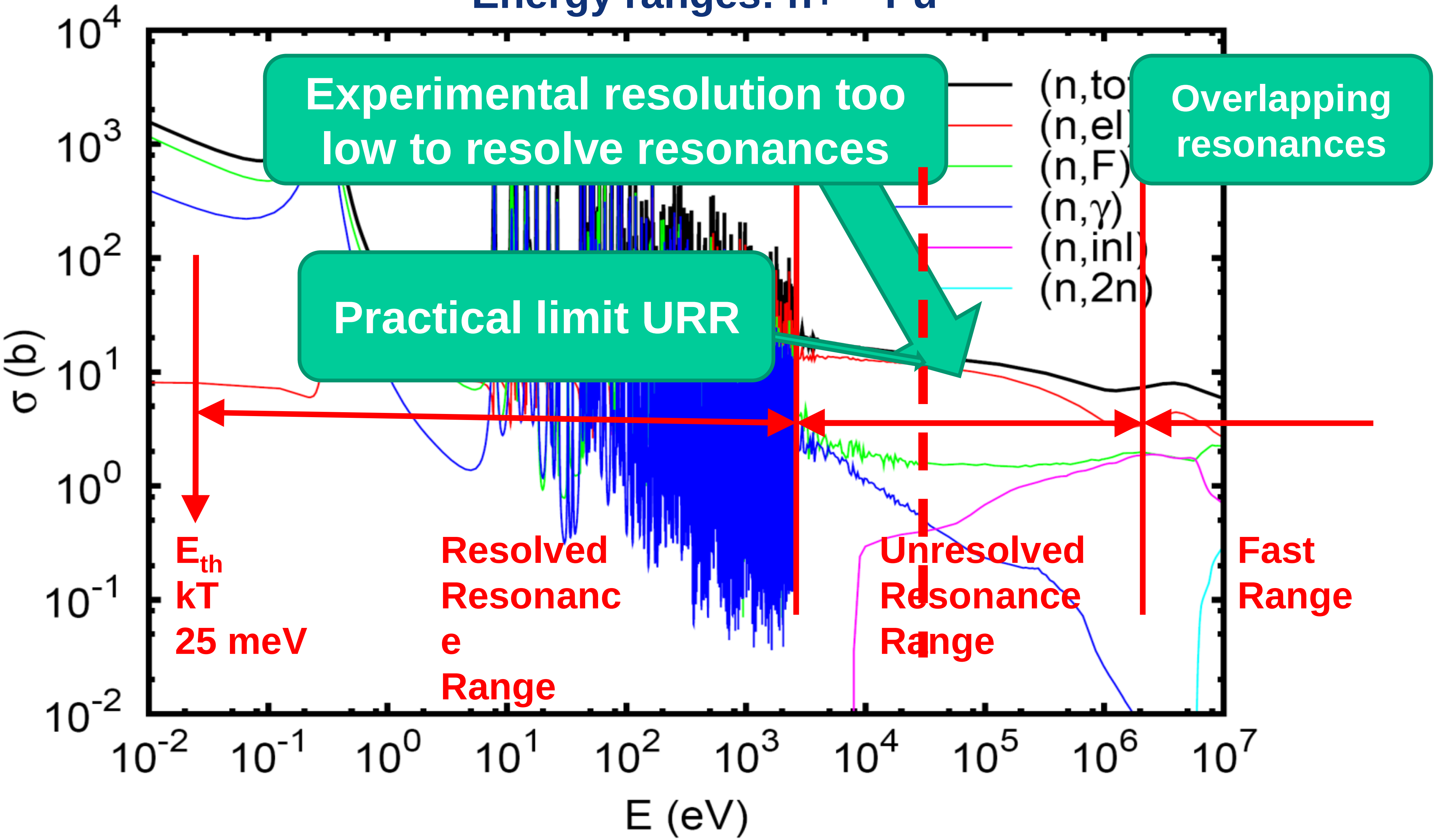
$$\sigma_T(E) = g_J \frac{4\pi}{k^2} \left\{ \frac{\Gamma_n \Gamma/4}{(E - E_0)^2 + \Gamma^2/4} + \frac{\Gamma_n (E - E_0) k R'}{(E - E_0)^2 + \Gamma^2/4} + (kR')^2 \right\}$$

Radius

Many parameters
E_0, J^π, Γ, Γ_n, Γ_γ, Γ_f, R', g_J
R-matrix: sophisticated model
Advanced analysis codes:
REFIT, SAMMY, CONRAD

Characterization of resonances requires measurements with good energy resolution
Good understanding of broadening mechanisms

Energy ranges: n+^{239}Pu



Summary part 1

Data of interest
Use of uncertainties
Need for measurements

Cross section

total, fission, elastic
inelastic, residual or
ejectile yields

Differential cross section

- Angular distribution
- Emission spectrum
- Double differential

Other parameters

Resonance parameters

Influence quantities

Doppler broadening
Instrumental broadening
Sample broadening
Temperature
Pressure
Sample composition, impurities,
dimensions, roughness,…
Room return
Collimation
Neutron sources