Hybrid R-Matrix Evaluation of Neutron-Induced Reaction Cross Sections of O-16

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Work partly supported by EUROfusion Engineering Grants, Work Package Materials

1. Introduction

Evaluations of light nuclear systems are not straightforward at present

- The resonance range goes up to incident energies beyond 10 MeV
- Available (semi-)microscopic models are insufficient for quantitative description
- Application of the statistical model, if possible, only at sufficient high energies
- Opening of breakup channels at rather low energies in the resonance regime

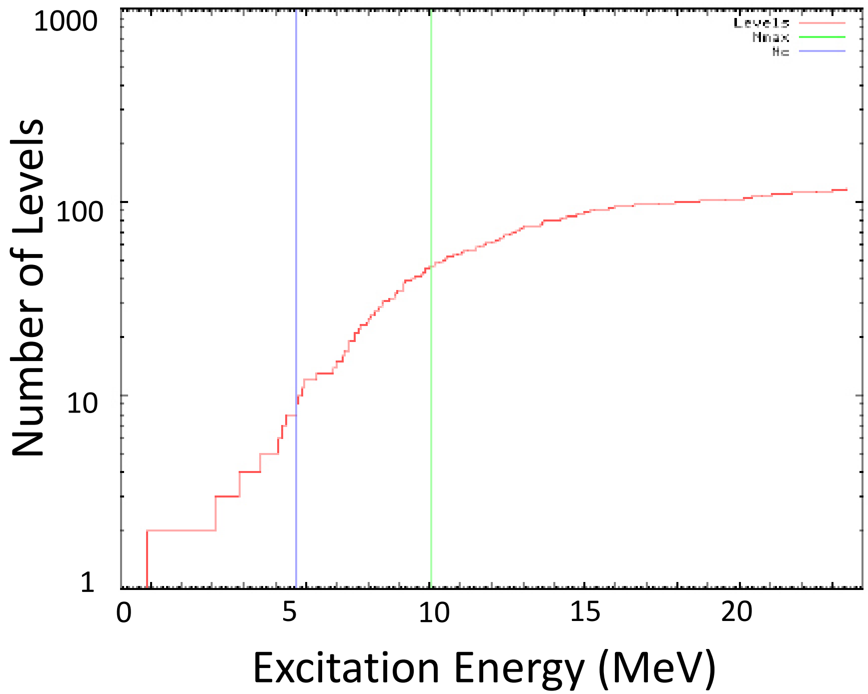
The ^{17}O Compound System

In light systems the level density of the compound nucleus is small

With increasing excitation energy the spectrum of the compound nucleus becomes more dense

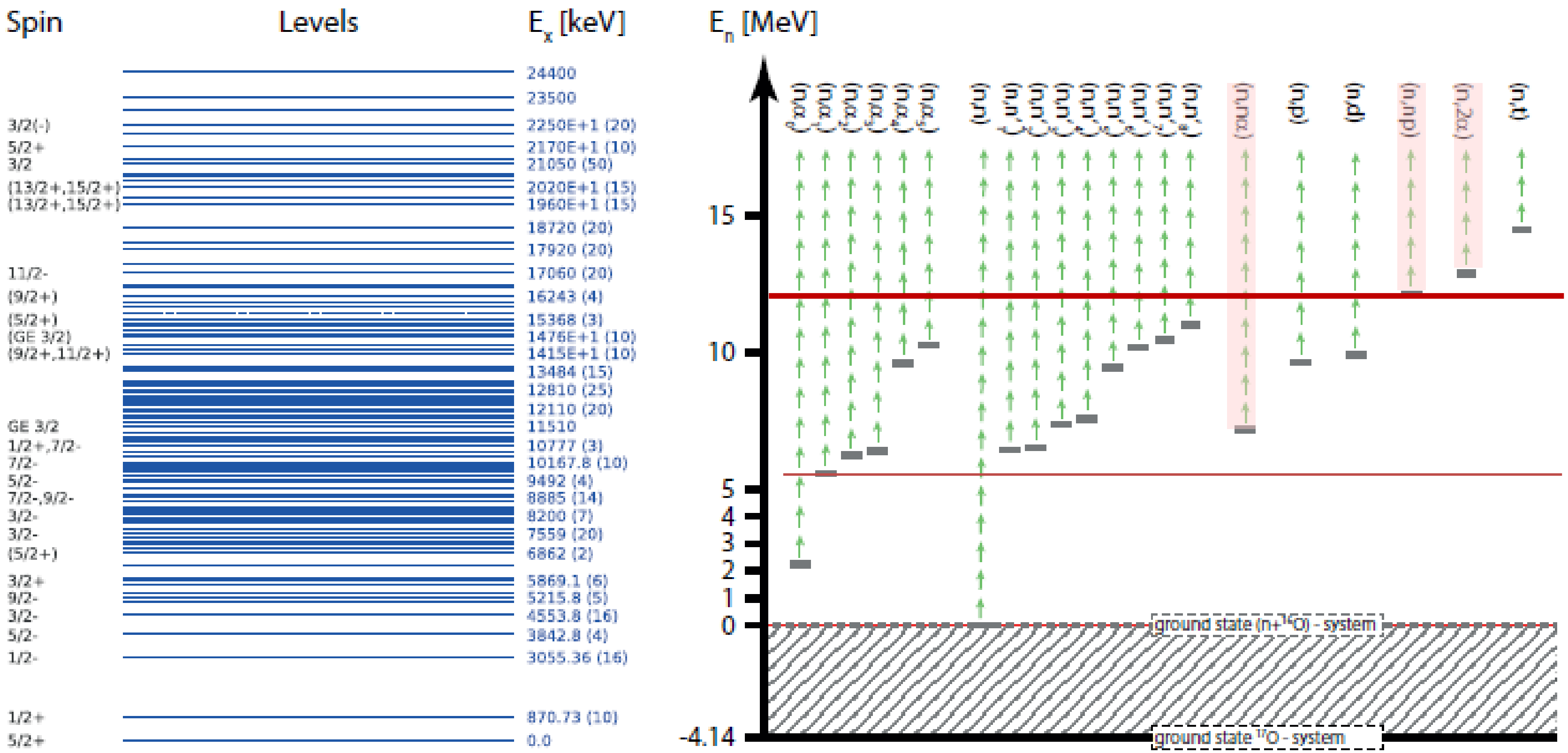
The statistical model might be successfully applied beyond a certain energy E_{cont}

cumulative discrete levels in compound nucleus ^{17}O



For the ^{17}O compound nucleus E_{cont} is between 10 and 15 MeV

The ^{17}O Compound System



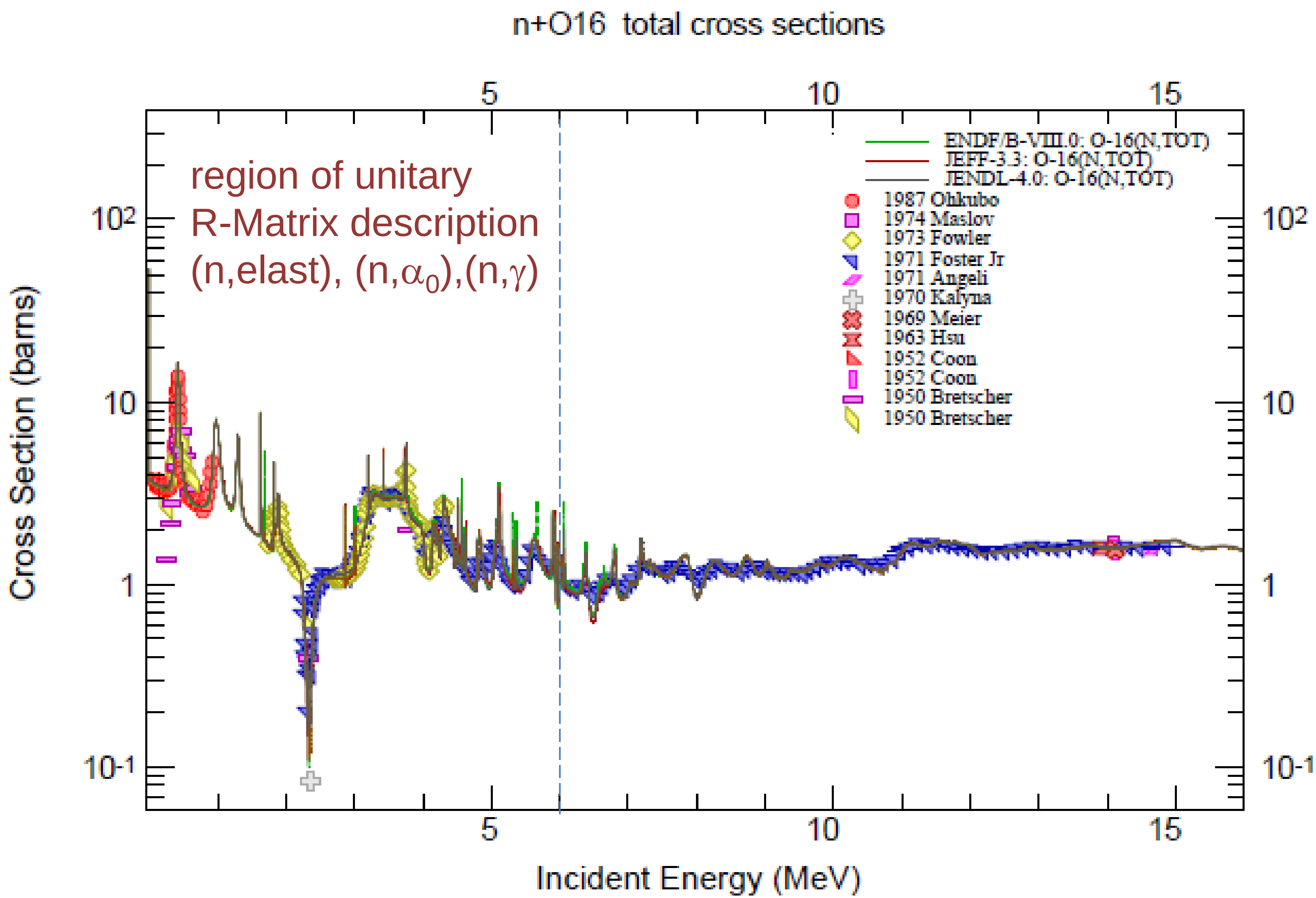
compound nucleus ^{17}O

possible decompositions up to 13 MeV

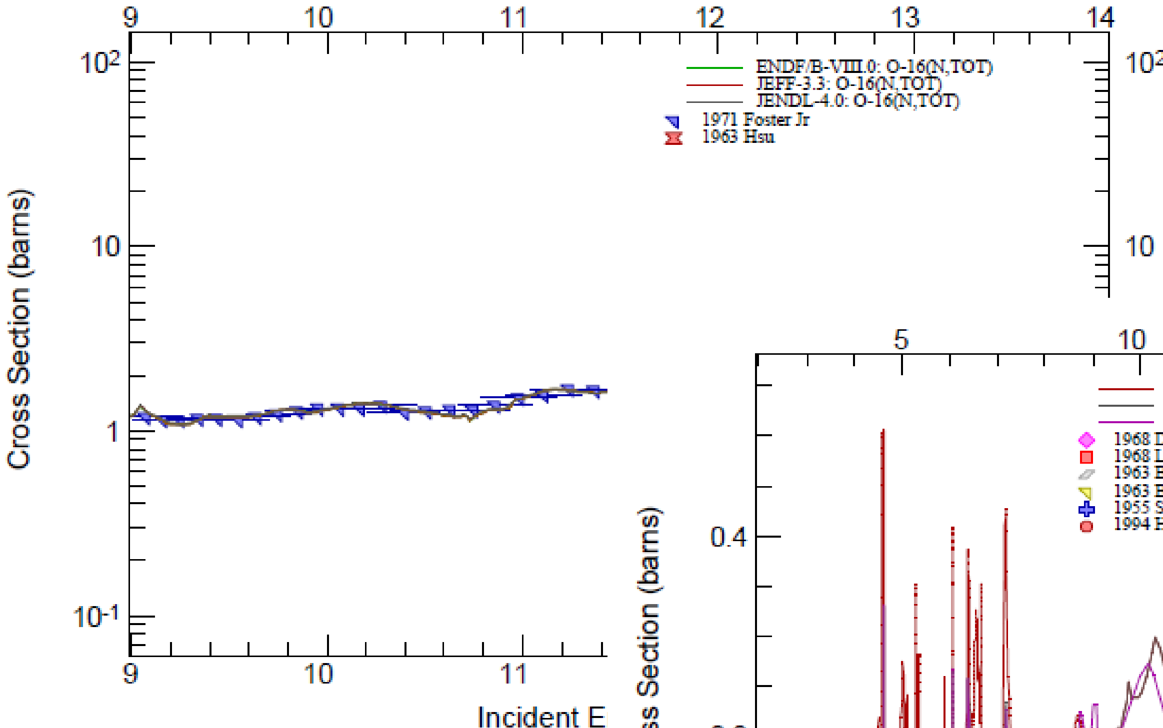
^{17}O, n+^{16}O, α+^{13}C, p+^{16}N, d+^{15}N

Unitary R-matrix calculations are currently performed only up to E_n ~ 5.6 MeV in cm system

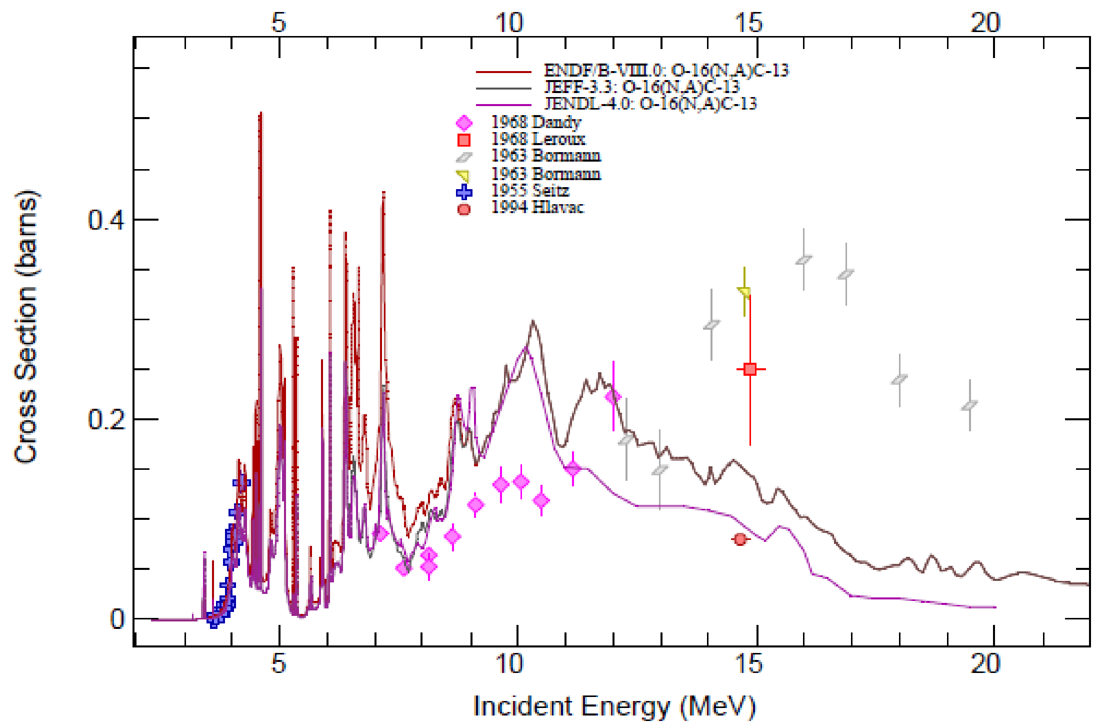
Evaluated neutron-induced reactions data on ^{16}O in the nuclear data libraries



Comparison of Nuclear Data Files for Neutron-Induced Reactions on ^{16}O



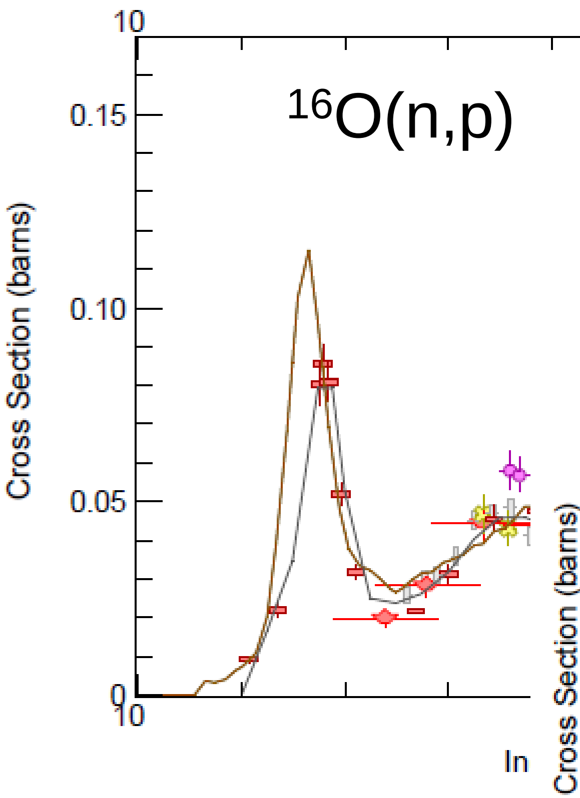
ENDF/B-VIII.0
JEFF 3.3
JENDL 4.0



total n-^{16}O cross section

Comparison of (n,α_0) cross section

Comparison of Nuclear Data Files for Neutron-Induced Reactions on ^{16}O



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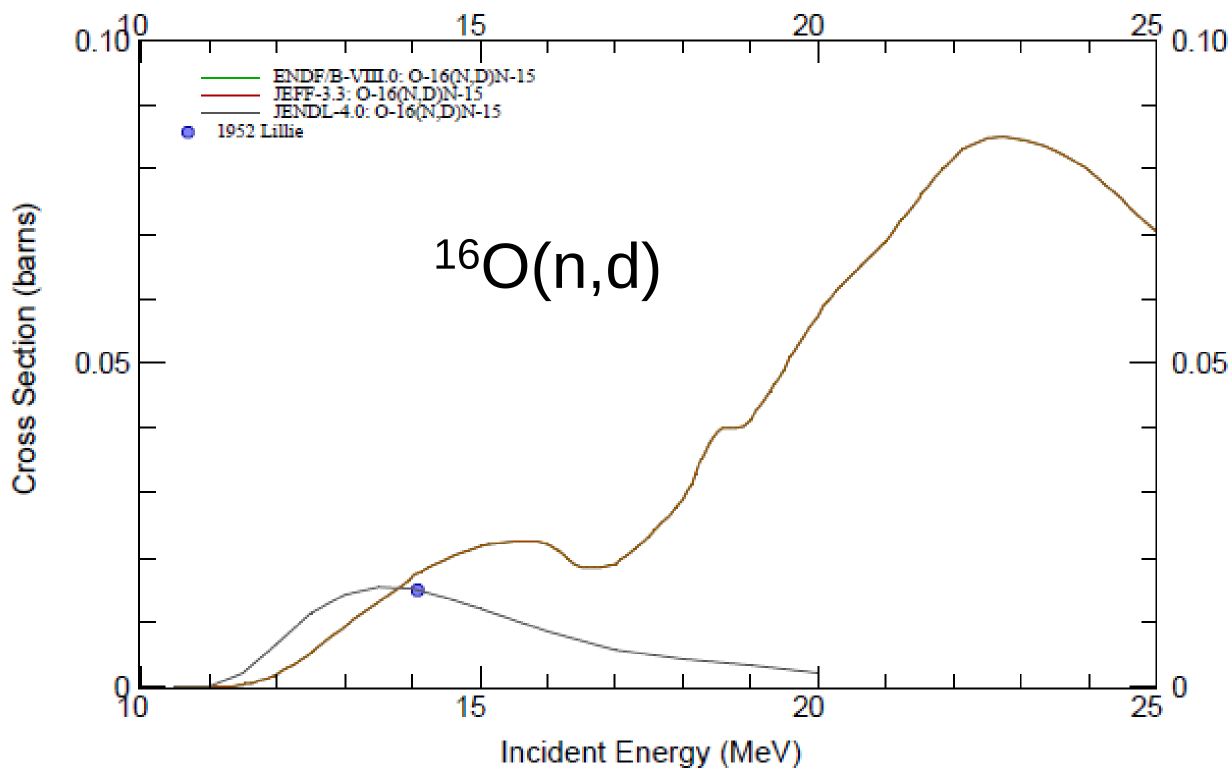


CIELO
New evaluation of $n+^{16}O$

Motivation of a new n-^{16}O Evaluations

- Oxygen is an important ingredient in many structure materials
- Current evaluations are not fully satisfying → CIELO project provided new evaluations, but there are still open problems → INDEN project
- Reliable uncertainty estimates are not available

Goals

- ➢ continuous transition between statistical model regime and resonance region
- ➢ unified evaluation over the whole energy region up to about 200 MeV
- ➢ accounting for model defects in the resonance regime
- ➢ extraction of consistent error bands and reliable covariance estimates
- ➢ attempts towards more microscopic understanding of resonance regime

Hybrid R-Matrix Approach:
Concept

Basic Properties:

- background poles are based on a realistic background potential (related to optical potentials used in statistical model calculations)

$$V_{\text{pseudo}}^{\text{back}}(r) \quad \Rightarrow \quad R_{cd}^{\text{back}}(E) = \sum_{\lambda} \frac{\gamma_{\lambda c}^{\text{back}} \gamma_{\lambda d}^{\text{back}}}{E_{\lambda}^{\text{back}} - E}$$

- continuous transition between R-matrix and statistical model regimes
- modification of background by additional poles which may be associated with many-nucleon resonances

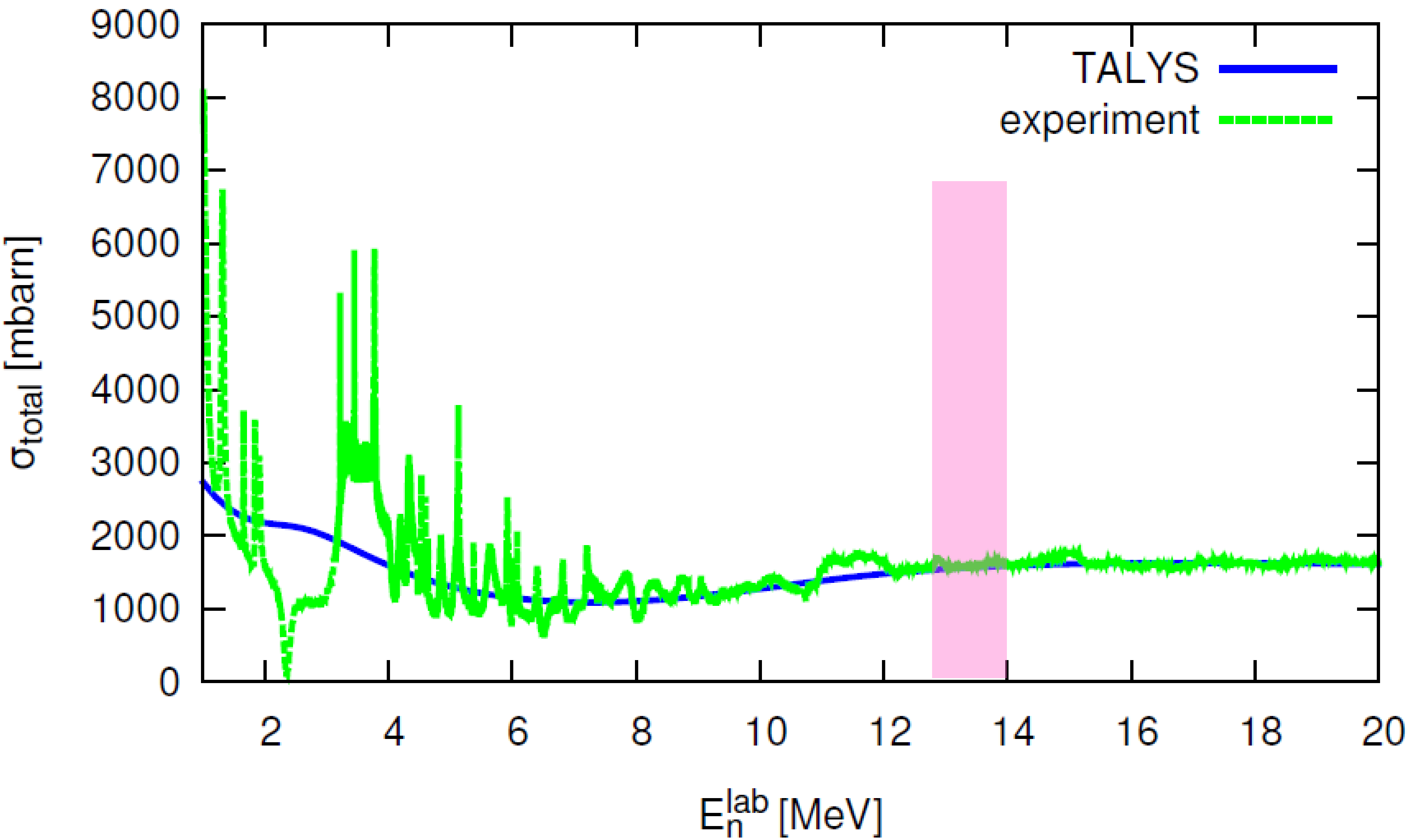
$$R_{cd}(E) = R_{cd}^{\text{back}} + \sum_{\lambda} \frac{\gamma_{\lambda c}\gamma_{\lambda d}}{E_{\lambda} - E}$$

background pseudo-potential expected to be smooth

pole terms should primarily describe many-body resonances

- use of a unique matching radius compatible with physics conditions

R-Matrix Theory and Statistical Model:
Matching the Theories



R-Matrix Theory and Statistical Model:
Matching the Theories

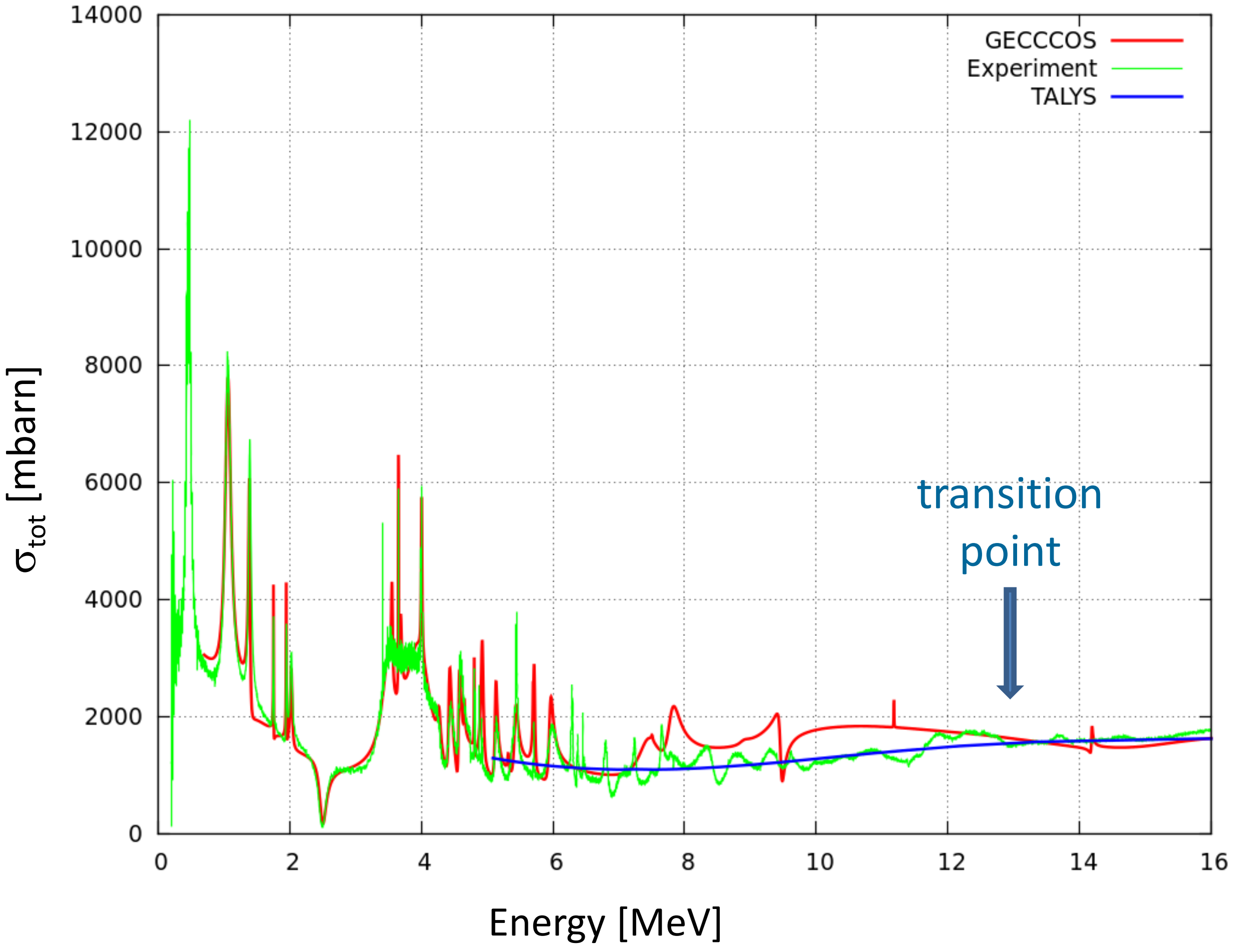
Coarse manual fit:

Match.Radius a=7 fm

Background plus
30 pole terms

partial waves J^{π}
$1/2^+$, $1/2^-$, $3/2^+$, $3/2^-$,
$5/2^+$, $5/2^-$, $7/2^+$, $7/2^-$,
$9/2^+$, $9/2^-$

sufficient up
to 15 MeV



R-Matrix Theory and Statistical Model:
Matching the Theories

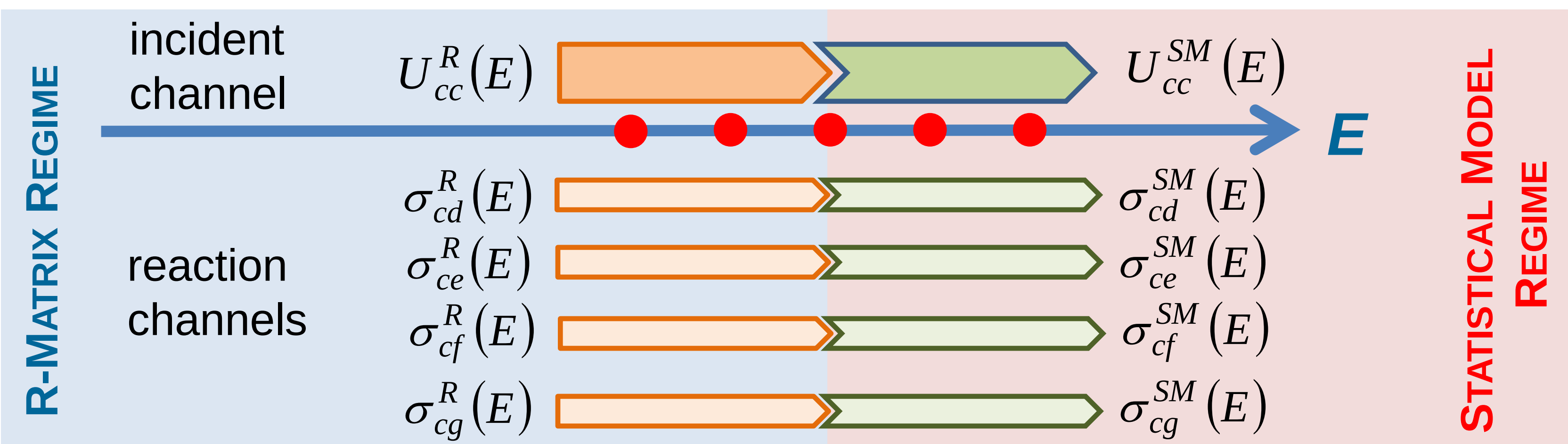
Concept of Statistical Model:

$$\sigma_{cd}(E) = \sigma_c^{\mathrm{CN}}(E) \times P_d^{CN}(E)$$

decay probability of CN into channel d

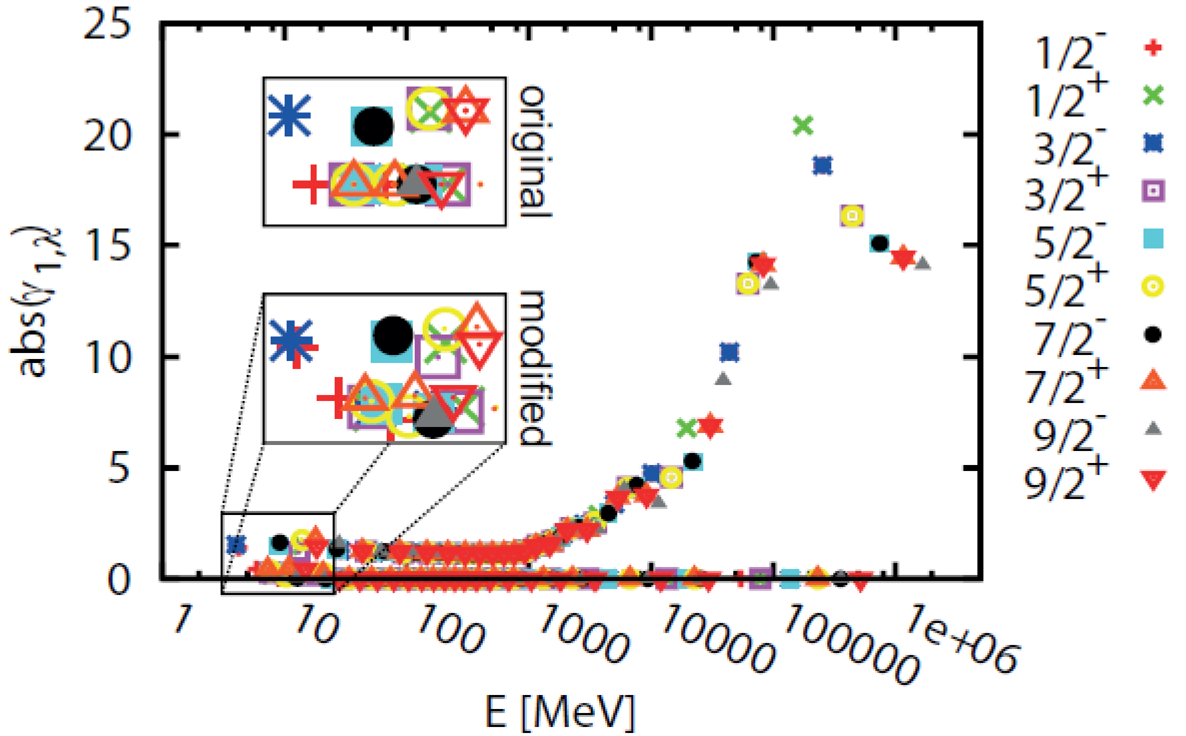
Formation cross section of CN

The statistical model only yields cross sections in reaction channels
S-matrix is known only for the incident channel for negligible compoundelastic contribution at the transition energy.



Matching: Statistical Model – *R*-Matrix Regime

Background Poles: Modifications



Optimization indicates that a spin-dependence of the background potential is required

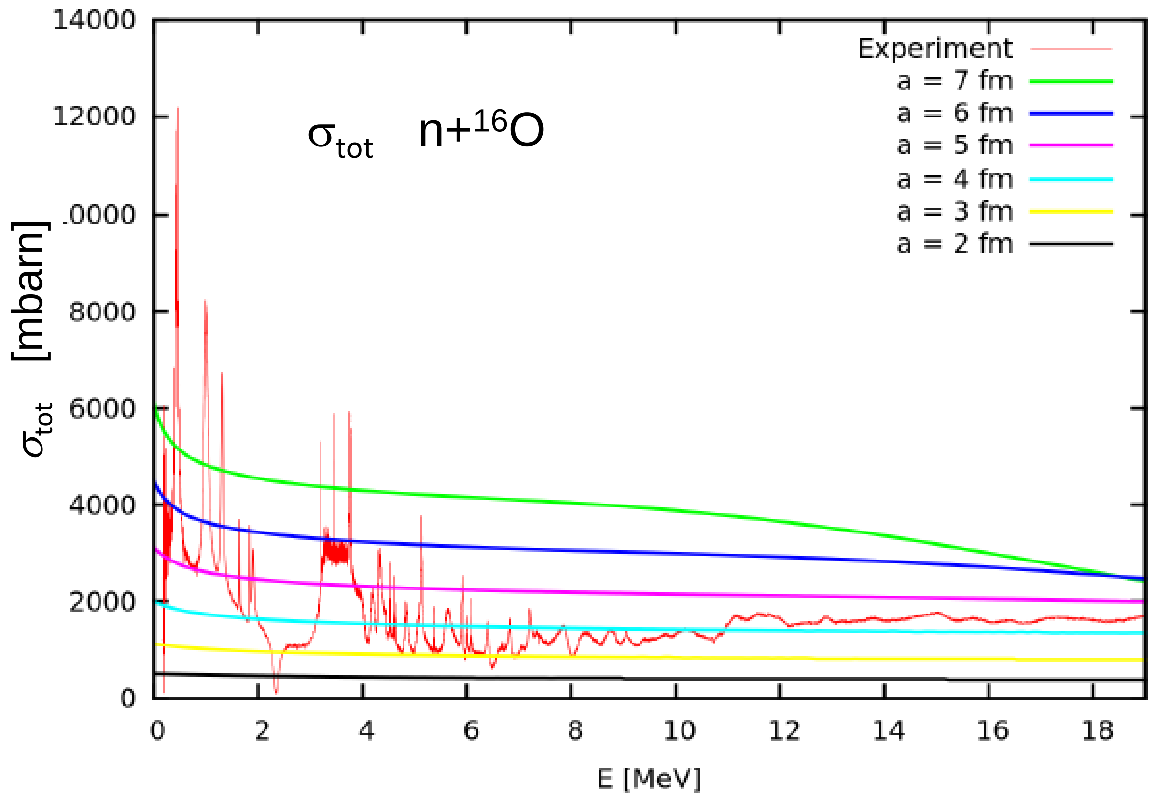
Problem: Matching Radius versus Physics

Physical matching radius
At light nuclei sufficiently small matching radius simplifies the pole fit of the data

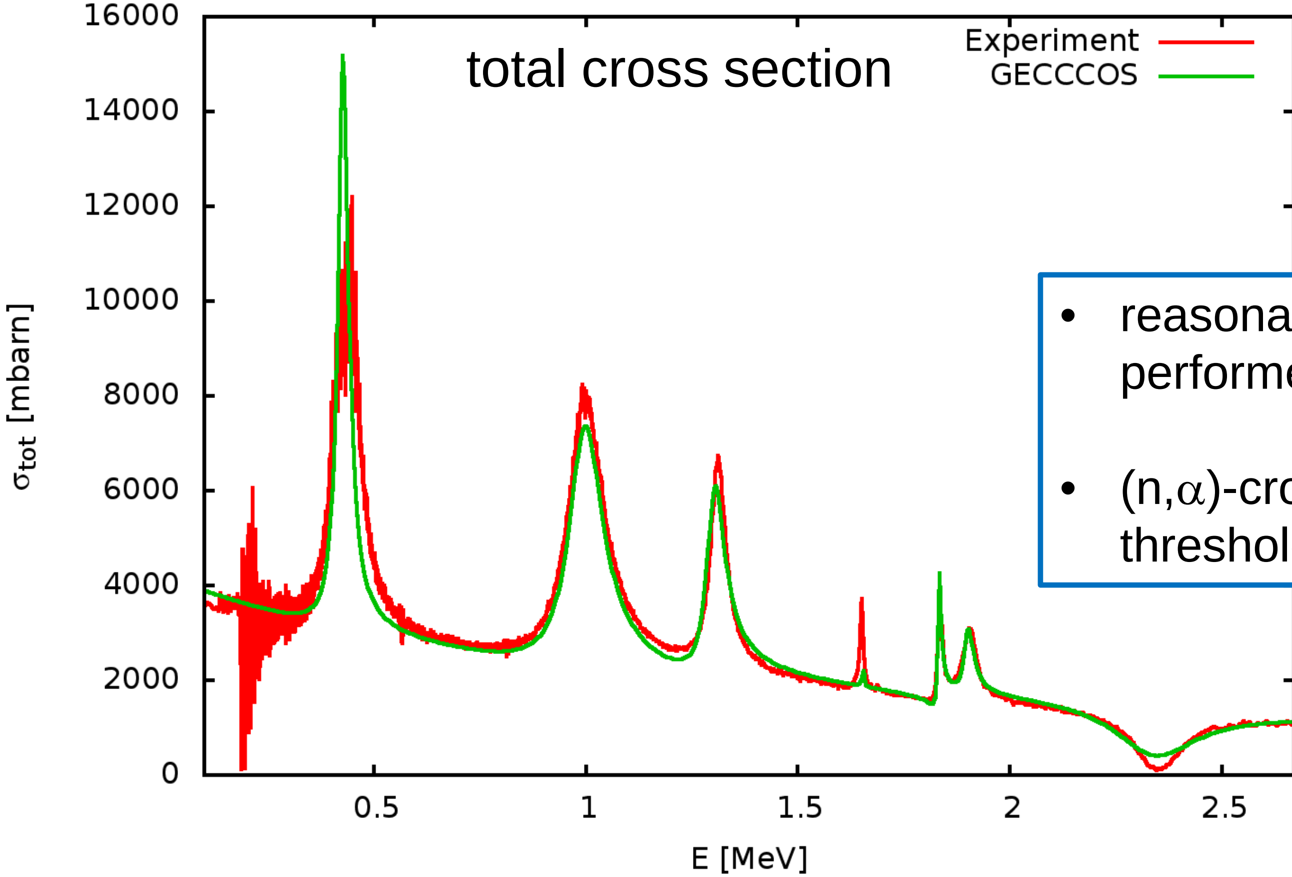
only few (1 to 2) back-ground poles suffice to mimic the background.

wave function is not physical nuclear potential for n+^{16}O extends to 6 -7 fm.

Example: CIELO evaluations use for n+^{16}O elastic channel a~3fm



n+^{16}O at 0.1 – 2.6 MeV



- reasonable fit (not perfect) performed with a = 2.8 fm
- (n,α)-cross section above threshold still negible

→ transform R-matrix from a = 2.8 fm to a = 7.0 fm possible?

S-Matrix equivalent R-Matrices for different matching radii

From *R*-matrix to the scattering matrix ***U*** in a coupled-channel system

$$\mathbf{U} = \mathbf{Z}_O^{-1}\mathbf{Z}_I$$

$$Z^O_{cd} = \frac{1}{\sqrt{k_a a}}\left[O_c(k_c a)\delta_{cd} - k_d a\, R_{cd} O'_d(k_d a)\right]$$

$$Z^I_{cd} = \frac{1}{\sqrt{k_a a}}\left[I_c(k_c a)\delta_{cd} - k_d a\, R_{cd} I'_d(k_d a)\right]$$

Determination of R-matrix from ***U***

$$\mathbf{R} = (\mathbf{OU} - \mathbf{P})(\mathbf{DU} - \mathbf{G})^{-1}$$

$$\mathbf{Z}_O = \mathbf{O} - \mathbf{RD}$$

$$\mathbf{Z}_I = \mathbf{P} - \mathbf{RG}$$

$\mathbf{D}, \mathbf{G}, \mathbf{O}, \mathbf{P}$ are known diagonal matrices

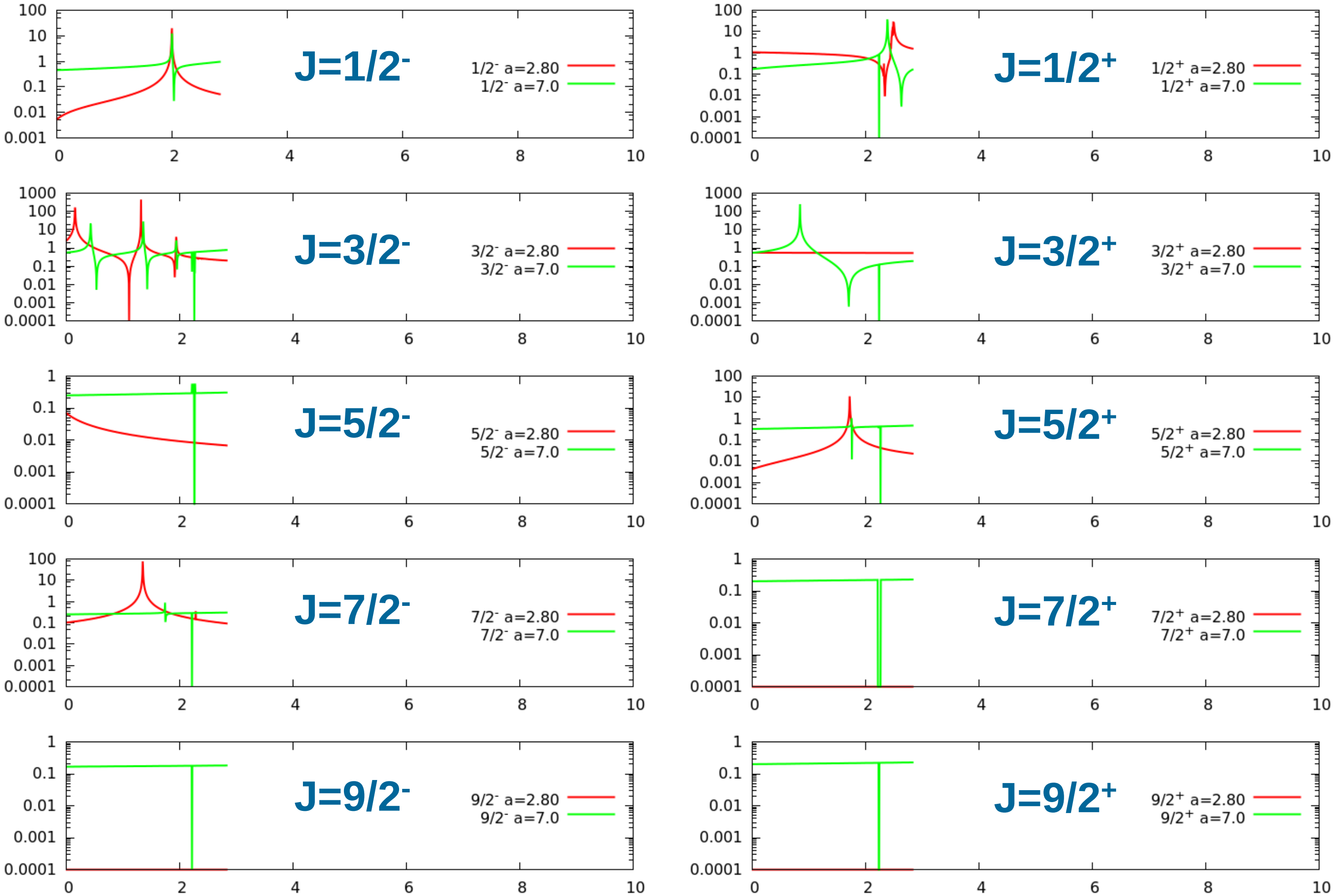
For hermitean Hamiltonians the resulting *R*-matrix must be again of the form

$$\mathrm{U}(\mathrm{E};\mathrm{a}_1) = \mathrm{U}(\mathrm{E},\mathrm{a}_2)$$

$$\mathrm{R}_{cd}(\mathrm{E};\mathrm{a}_1) = \sum_\lambda \frac{\gamma_{\lambda c}(\mathrm{a}_1)\gamma_{\lambda d}(\mathrm{a}_1)}{\mathrm{E}_\lambda(\mathrm{a}_1) - \mathrm{E}} \neq \mathrm{R}_{cd}(\mathrm{E};\mathrm{a}_1) = \sum_\lambda \frac{\gamma_{\lambda c}(\mathrm{a}_2)\gamma_{\lambda d}(\mathrm{a}_2)}{\mathrm{E}_\lambda(\mathrm{a}_2) - \mathrm{E}}$$

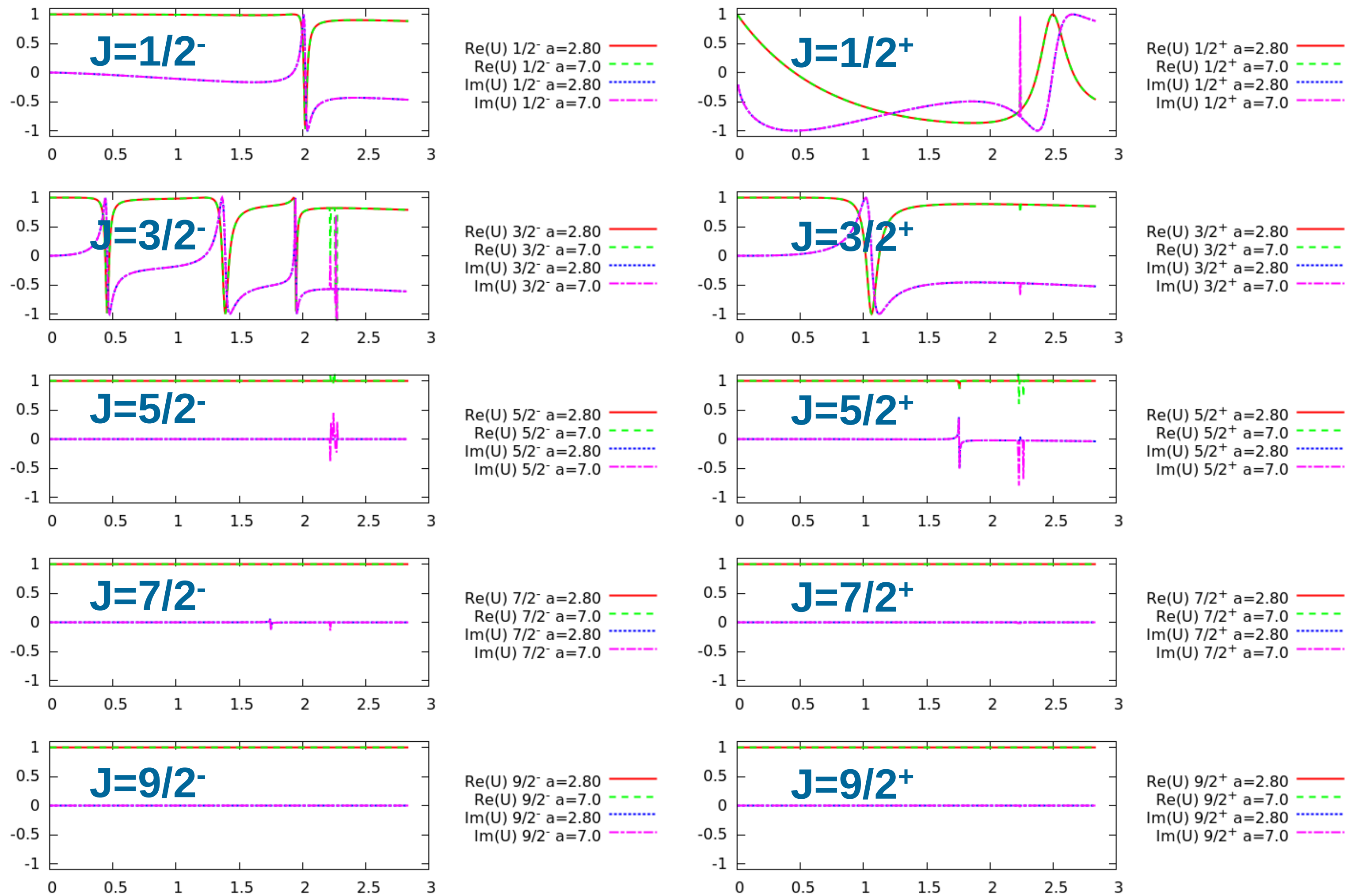
change of matching radius

Elastic R-matrix element per partial wave as function of Energy (a = 2.8 fm and a = 7.0 fm)

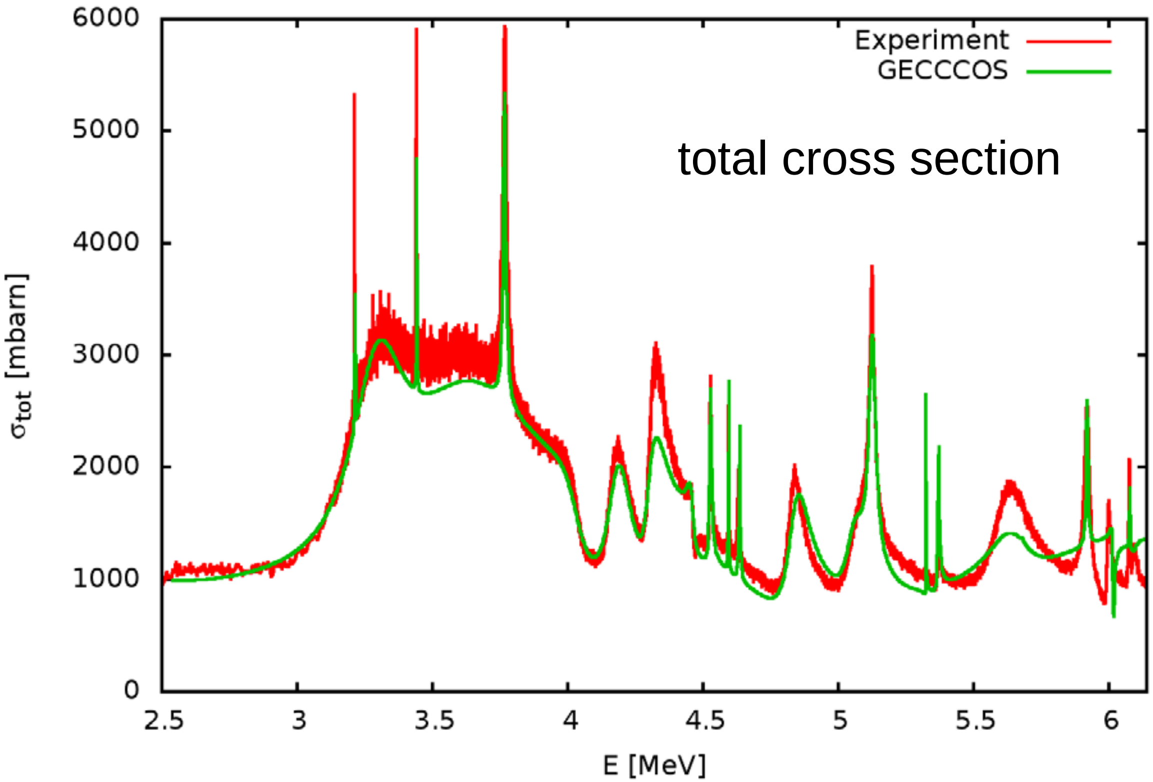


check U-matrix

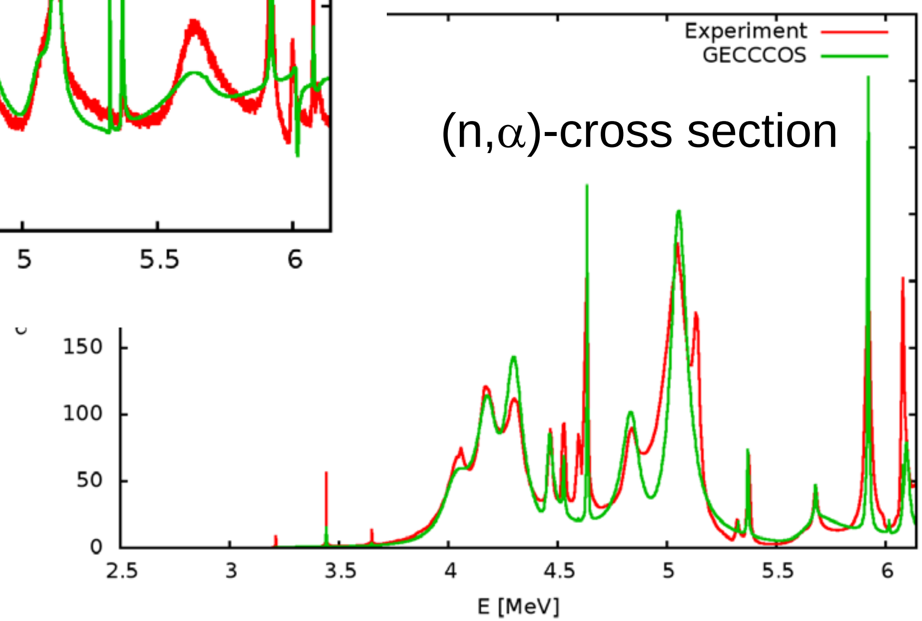
Elastic U-matrix element per partial wave as function of Energy (a = 2.8 fm and a = 7.0 fm)



n+^{16}O in the region 2.5 – 6.2 MeV



- pole fit (not perfect) done with a=3.27 fm



→ transform R-matrix from a = 3.27 fm to a = 7.0 fm

change of matching radius

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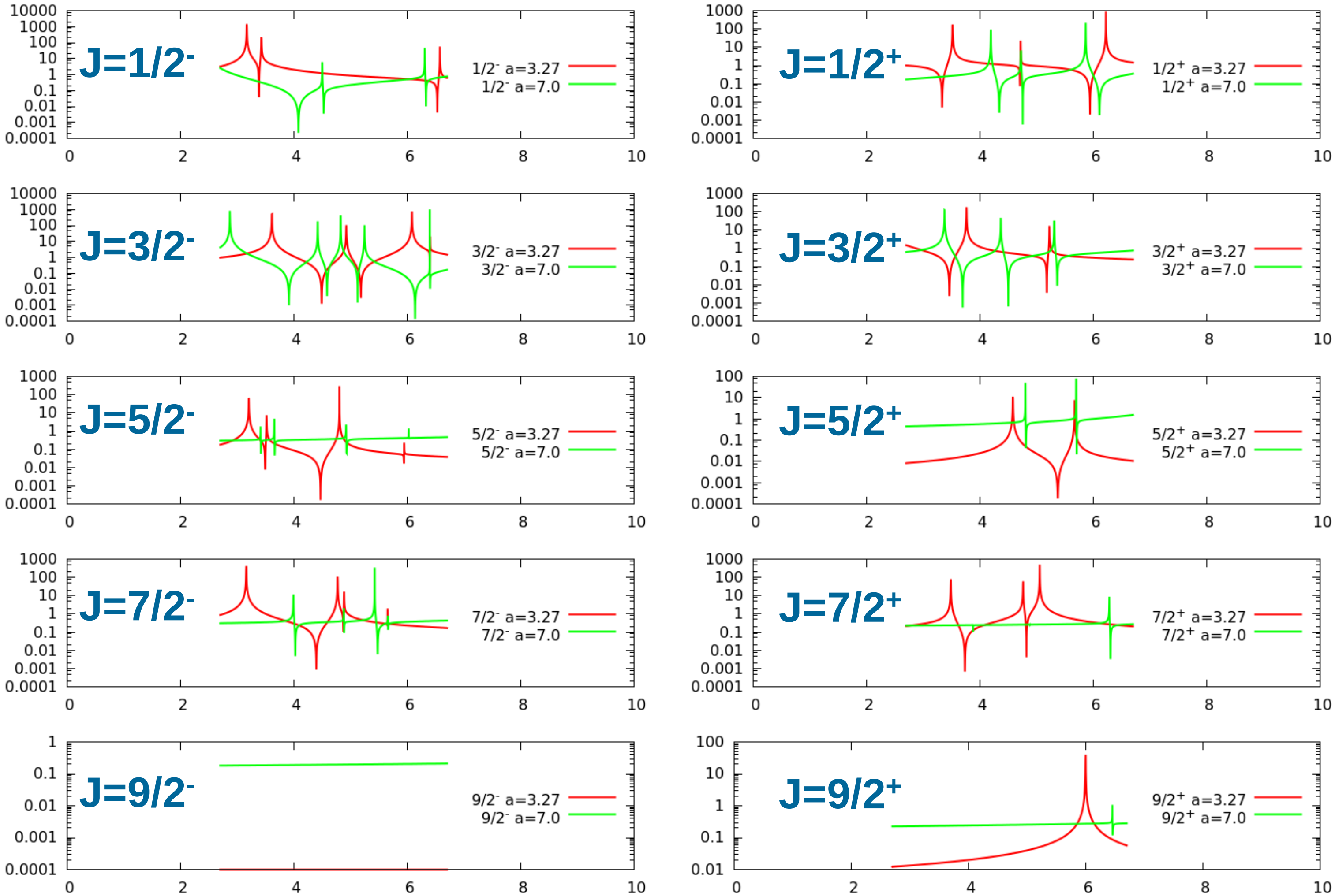
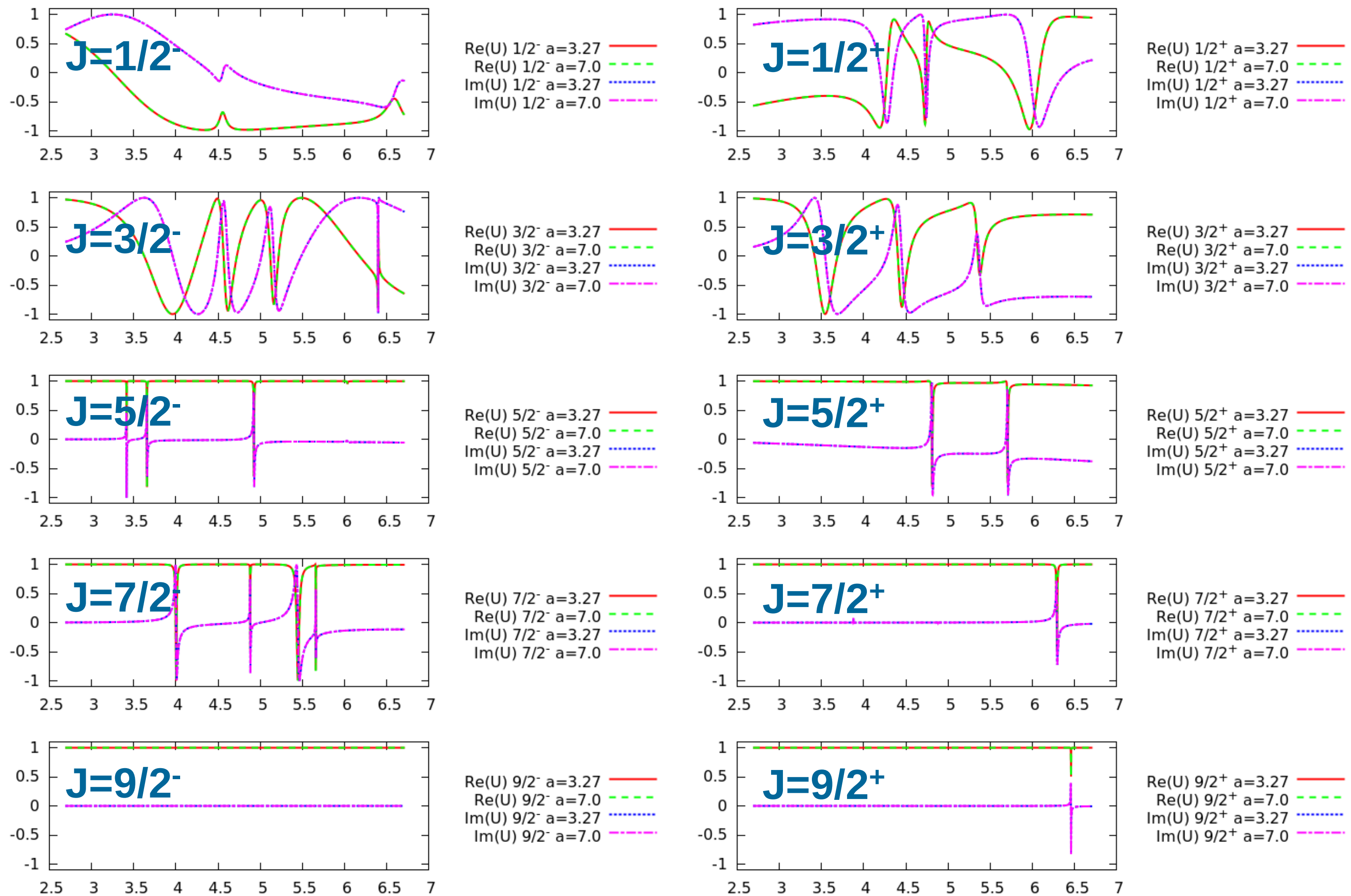
Elastic R-matrix element per partial wave as function of Energy (a = 3.27 fm and a = 7.0 fm)



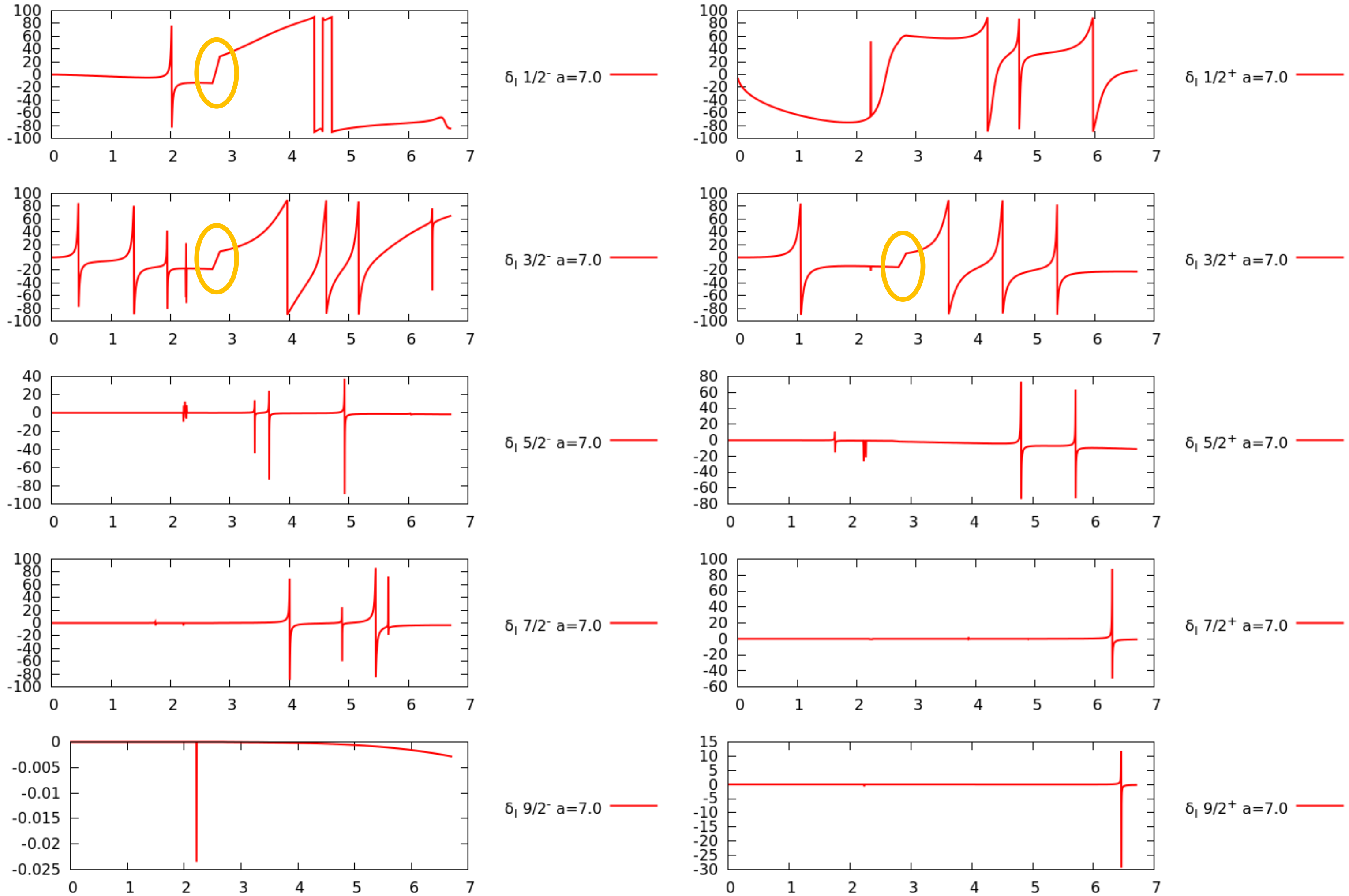
check U-matrix

Elastic U-matrix element per partial wave as function of Energy (a = 3.3 fm and a = 6.0 fm)



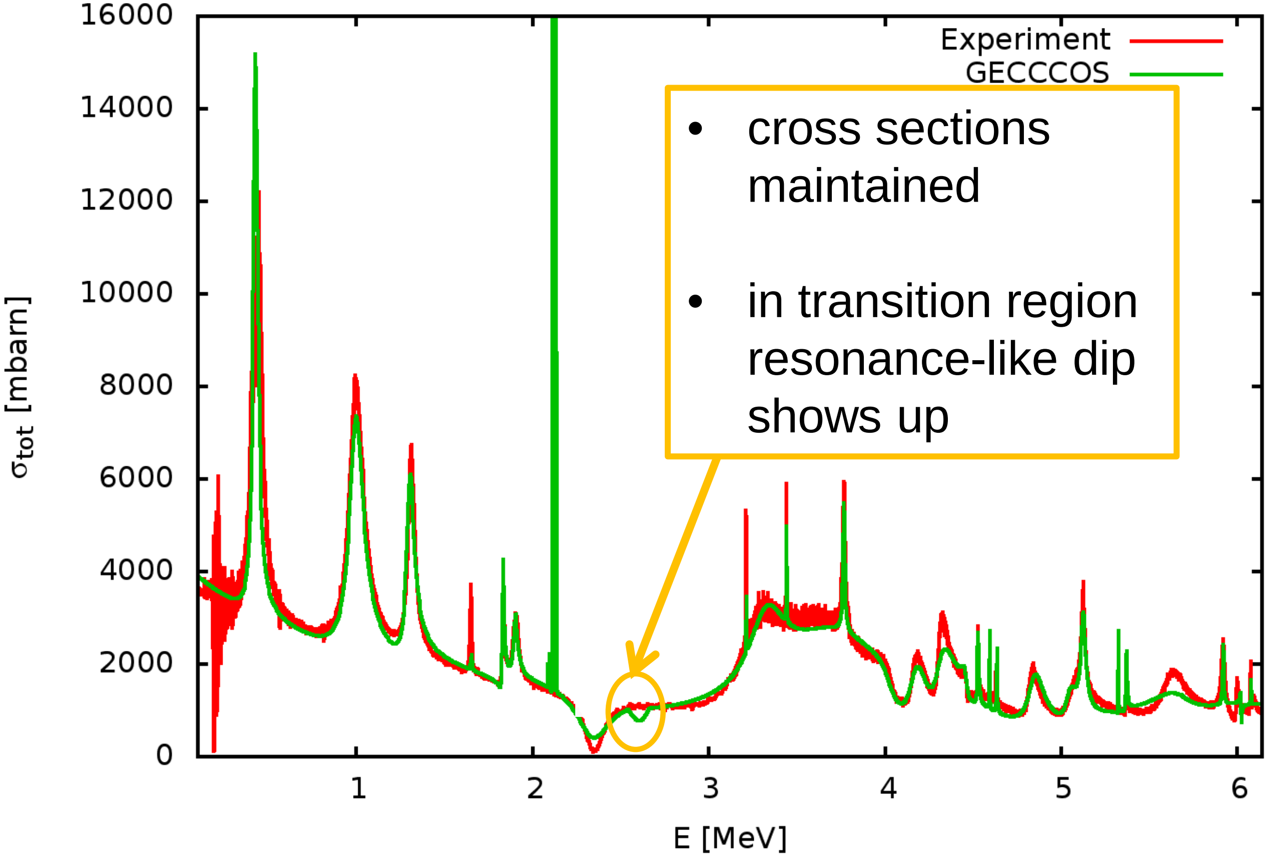
Phase shift δ_l at the intersection point

phase shift of elastic U-matrix element per partial wave as function of energy after blending overlapping energy regions



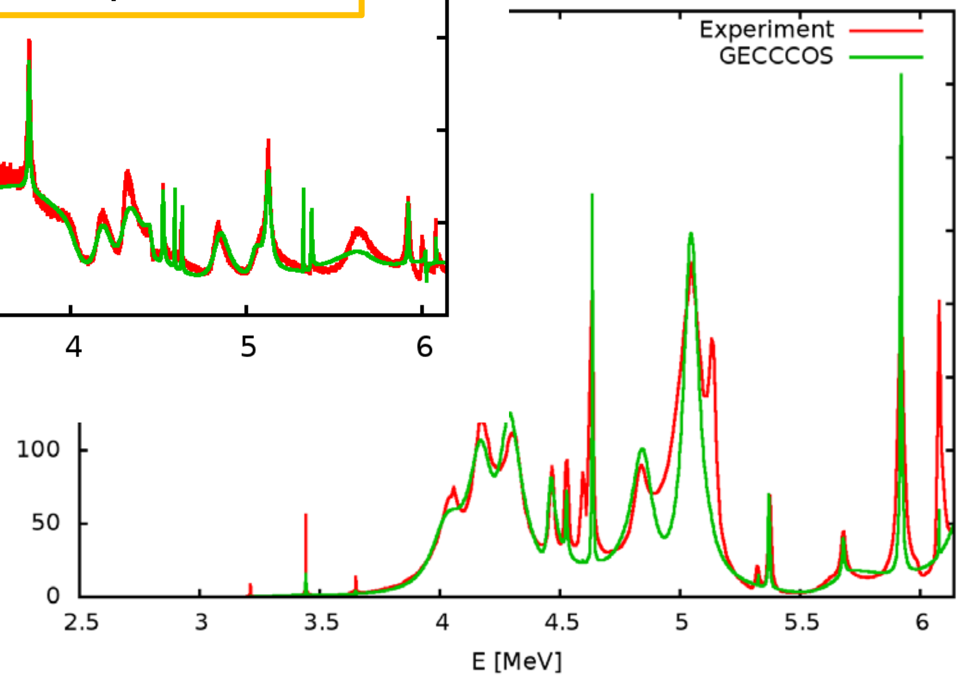
Reconstructed Cross Sections

total cross section



- cross sections maintained
- in transition region resonance-like dip shows up

(n,α)-cross section



Hybrid R-Matrix Approach on n+^{16}O
Open Reaction Channels

	Reaction	Q-value [MeV]	Threshold [MeV]		Reaction	Q-value [MeV]	Threshold [MeV]
	(n,γ)	4.219	0.000	y	(n,n'$_5$)	-8.872	9.431
y	(n,n)	0.000	0.000	y	(n,n'$_6$)	-9.585	10.189
y	(n,α_0)	-2.217	2.356	y	(n,n'$_7$)	-9.845	10.465
y	(n,α_1)	-5.306	5.641	y	(n,n'$_8$)	-10.356	11.009
y	(n,α_2)	-5.901	6.273		(n,nα)	-7.162	7.614
y	(n,α_3)	-6.070	6.453	y	(n,p)	-9.639	10.246
y	(n,α_4)	-9.081	9.653	y	(n,d)	-9.946	10.574
	(n,α_5)	-9.709	10.321				
y	(n,n'$_1$)	-6.049	6.431		(n,np)	-12.171	12.938
y	(n,n'$_2$)	-6.130	6.516		(n,2α)	-12.864	13.675
y	(n,n'$_3$)	-6.917	7.353		(n,t)	-14.520	15.436
y	(n,n'$_4$)	-7.117	7.566				

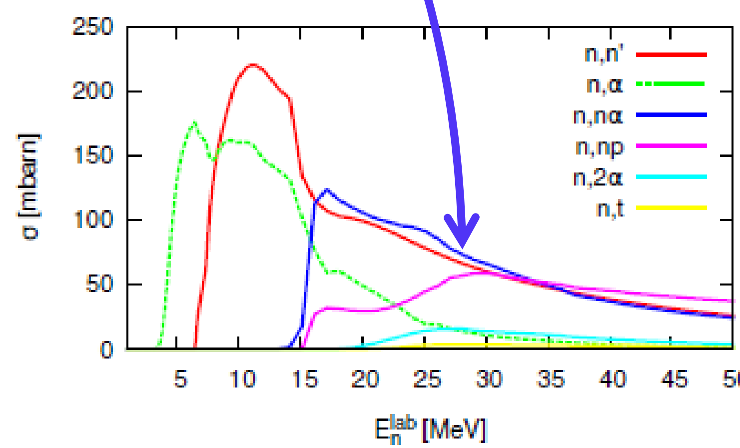
phase 2016

phase 2017

phase 2017

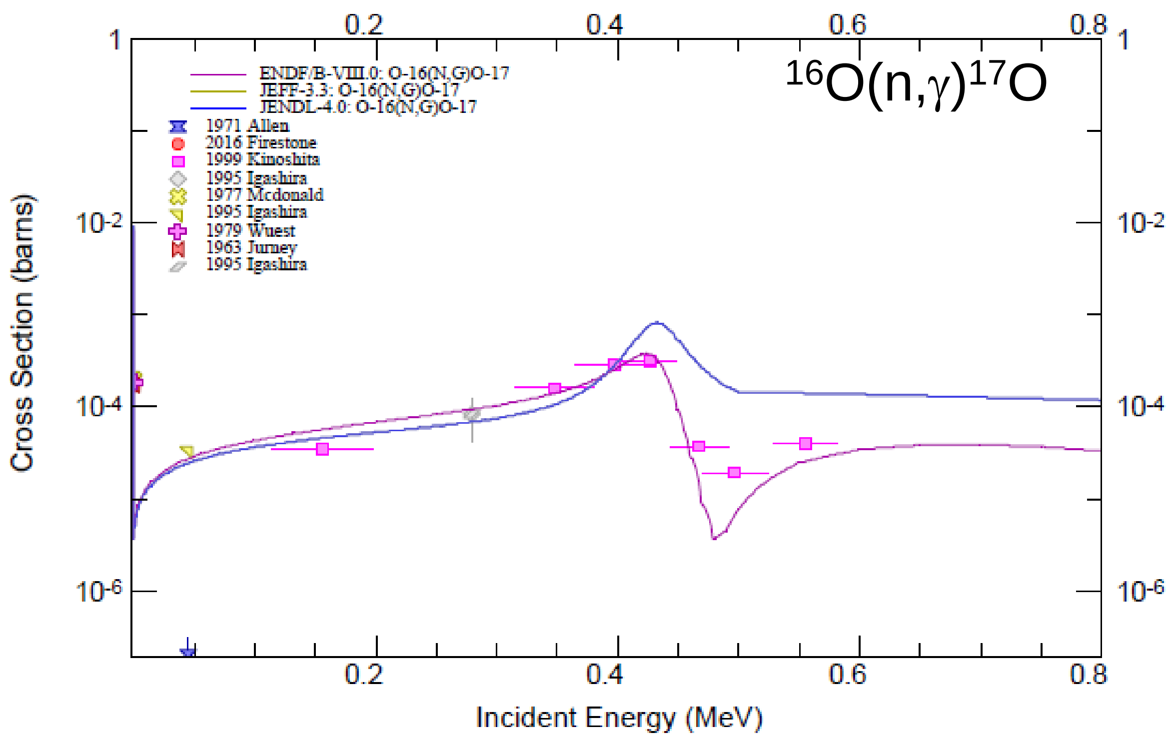
phase 2017

not a two-particle channel



Hybrid R-Matrix Approach for n+^{16}O:
Comment on (n,γ) capture reactions

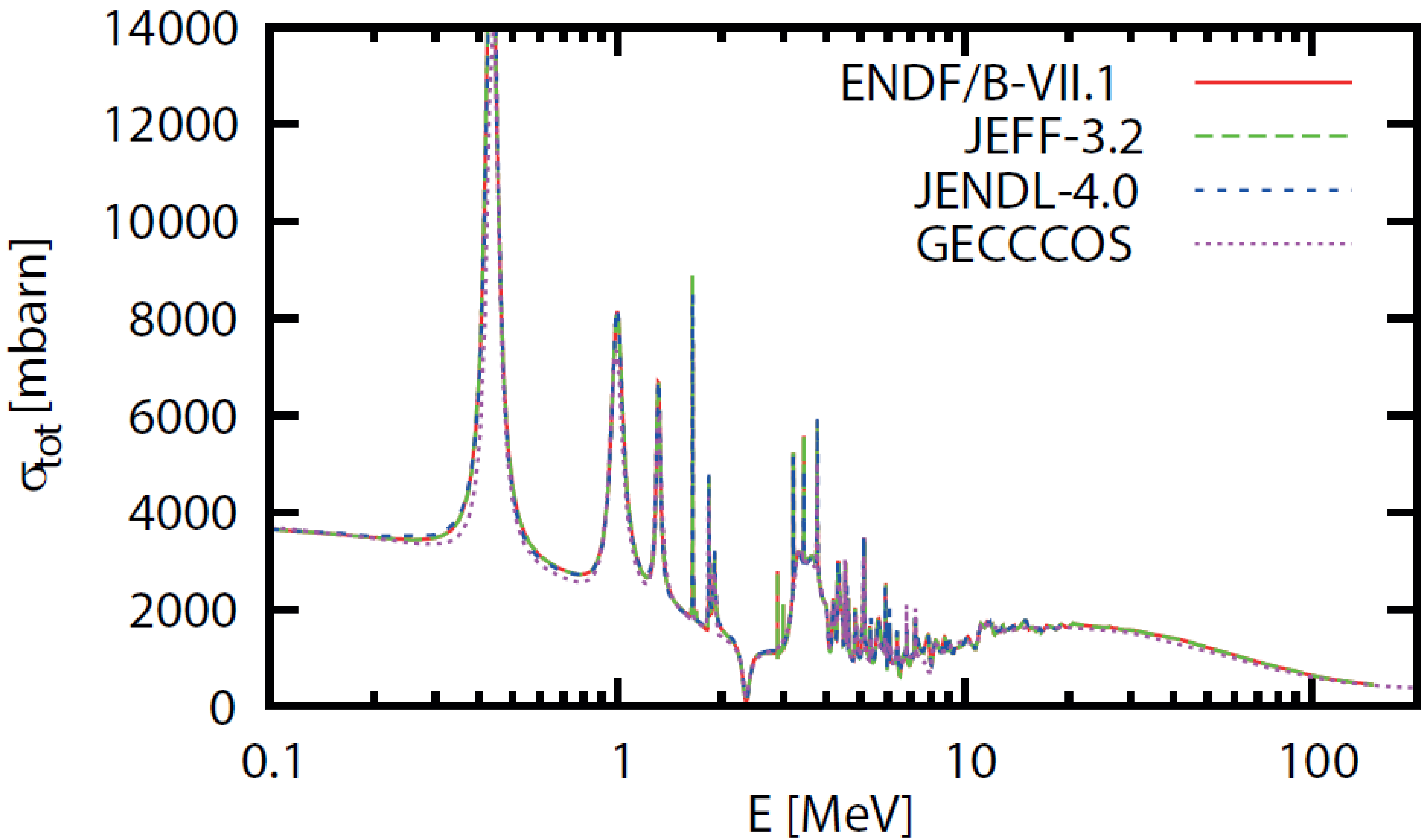
- R-Matrix theory inherently assumes binary particle channels.
- No natural description of capture channels → standard inclusion of capture channels via perturbative approach.



A unitary approach of (n,γ) reactions required

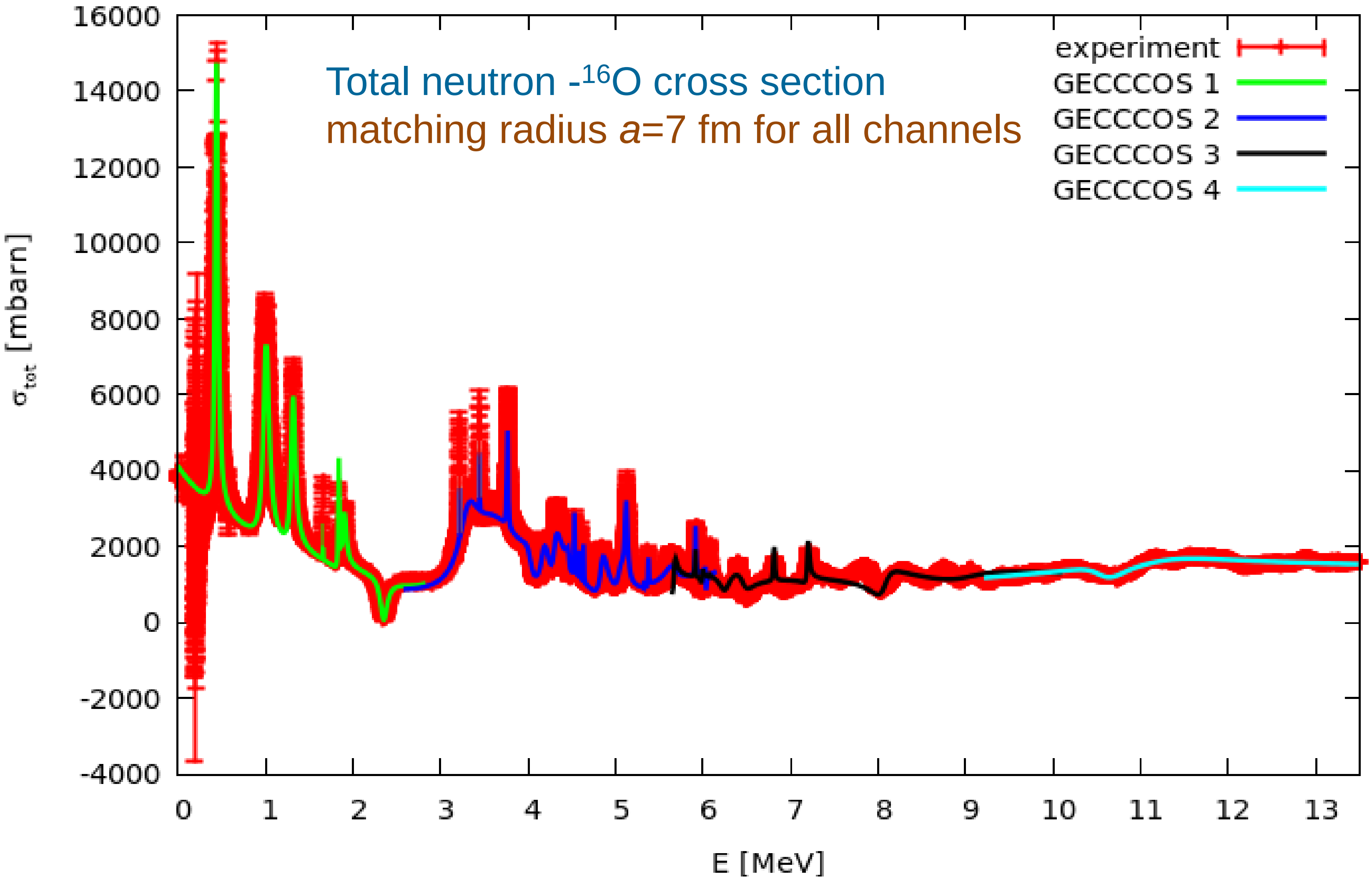
Ignoring (n,γ)-channels in the ^{17}O system results in less than 0.1% flux loss

Determining the best R-Matrix
Description of total cross sections

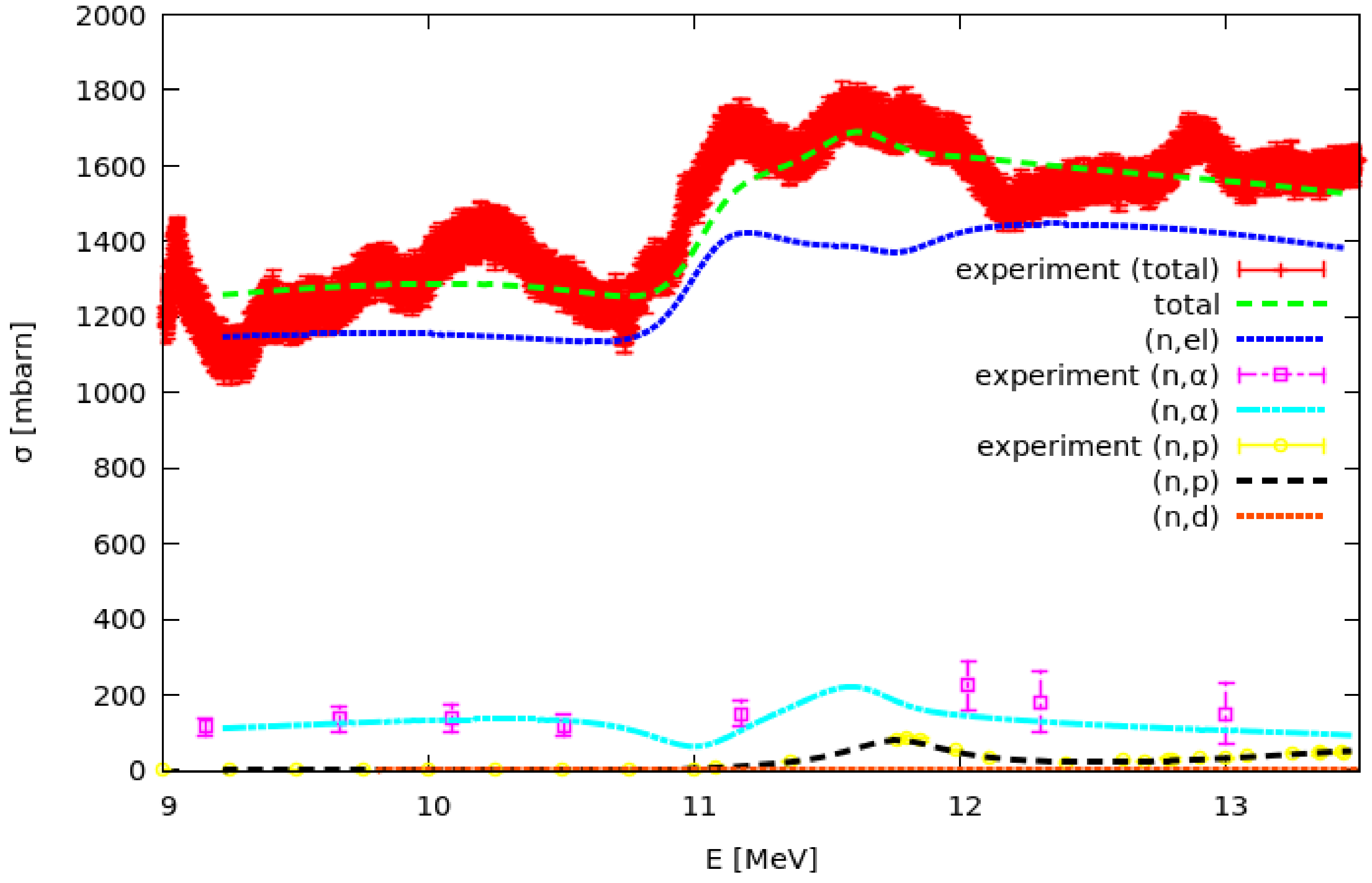


Determining the best R-Matrix

Description of total cross sections

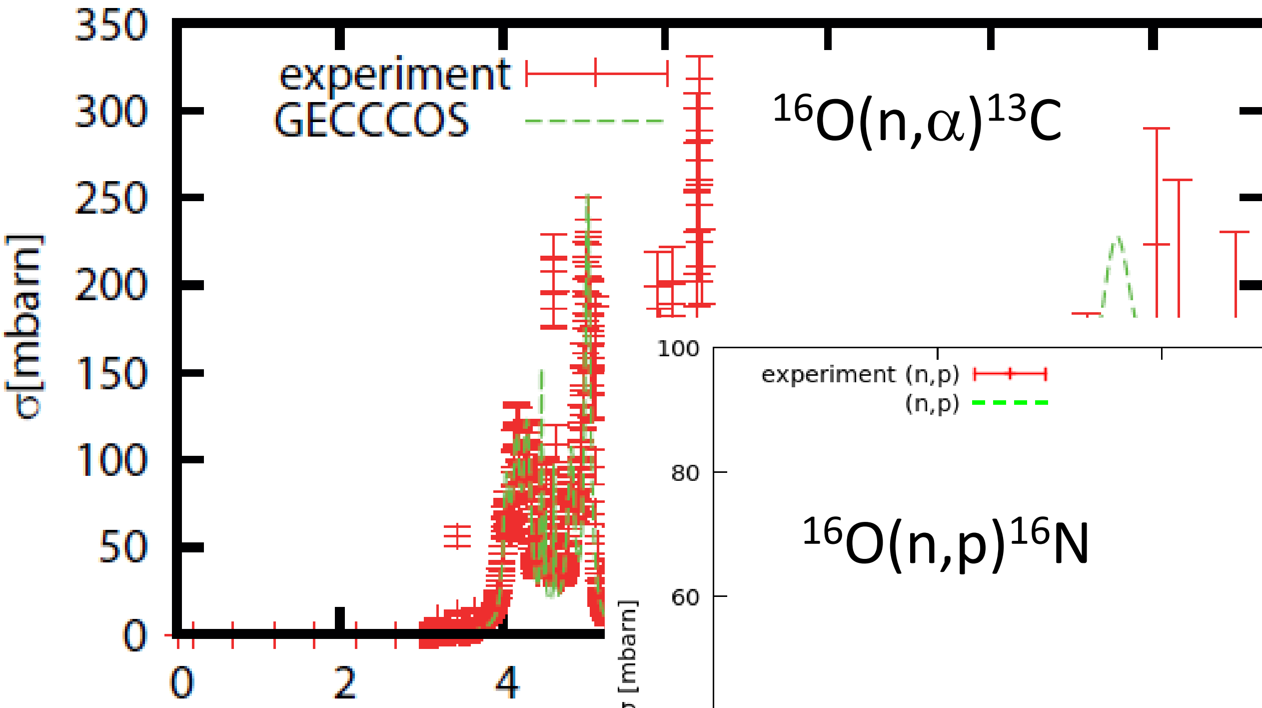


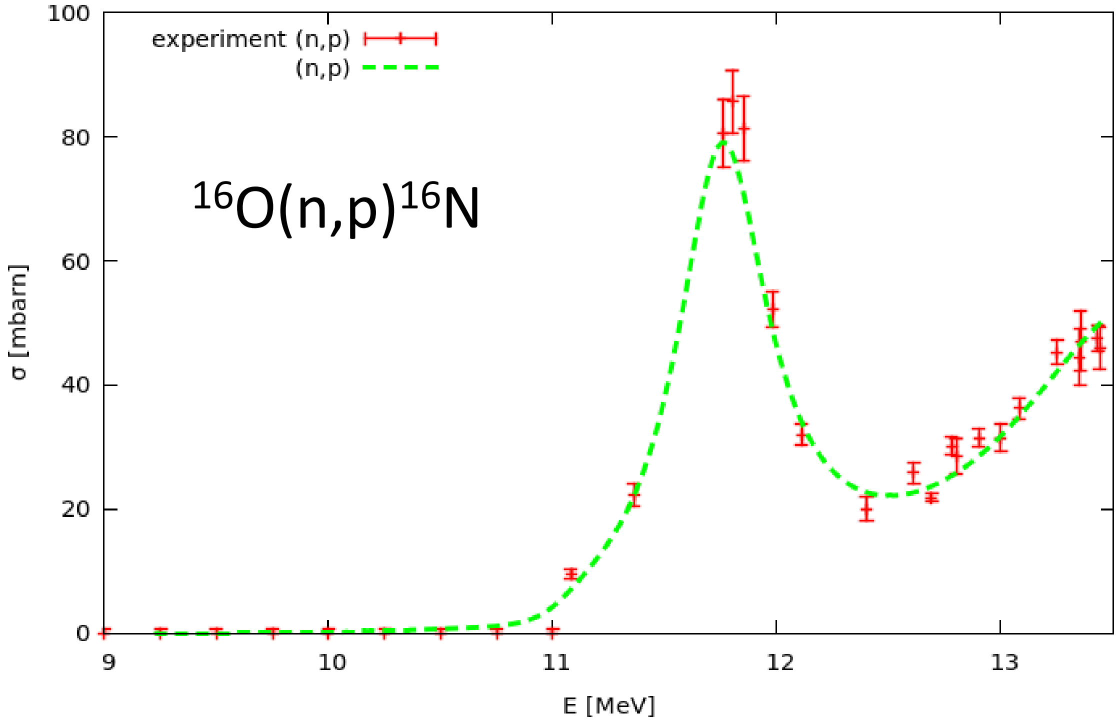
Determining the best R-Matrix
Comparison of Binary Cross Cections



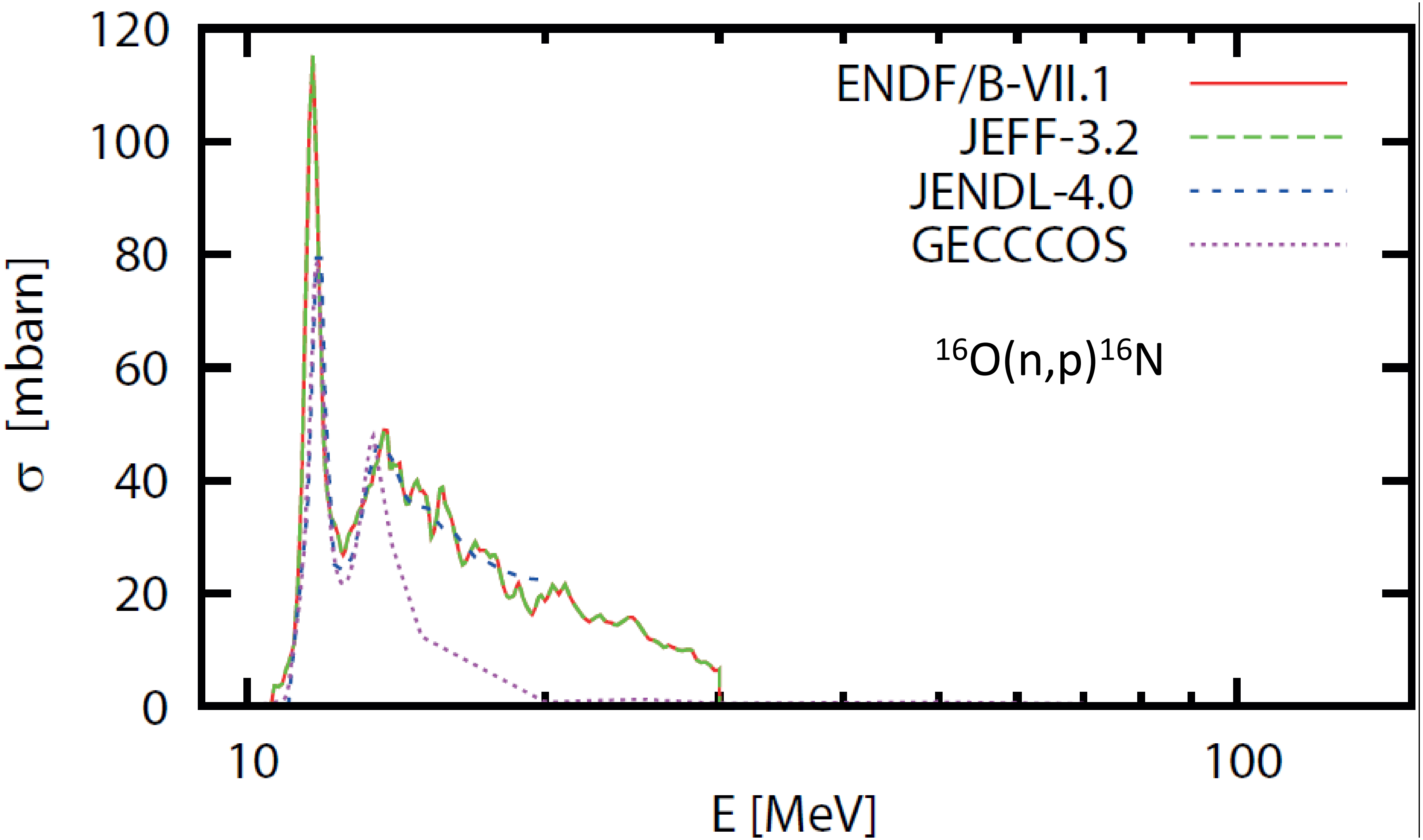
Determining the best R-Matrix

Description $^{16}O(n,\alpha)$ and $^{16}O(n,p)$ cross sections

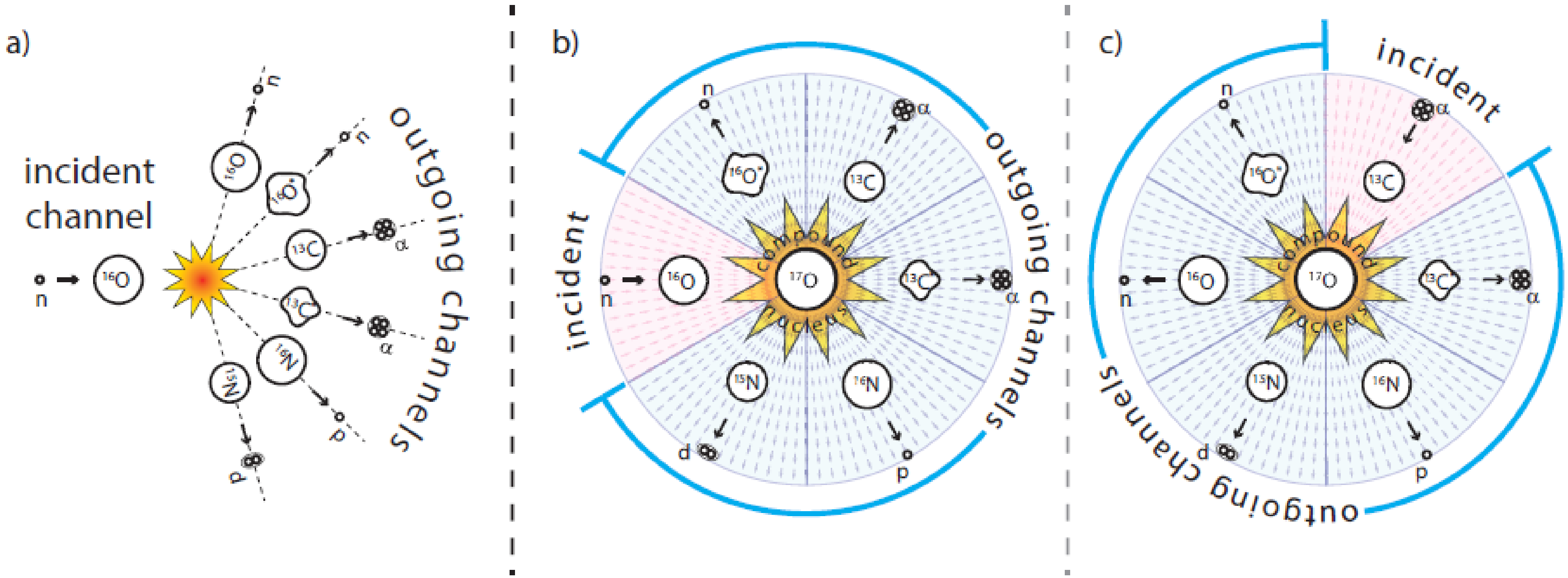




Determining the best R-Matrix
Description $^{16}O(n,\alpha)^{13}C$ cross sections



Evaluation of Light Nuclei Reaction Data
Compound Nucleus System



GECCCOS R-Matrix Module:
Towards a Tool for Analysis

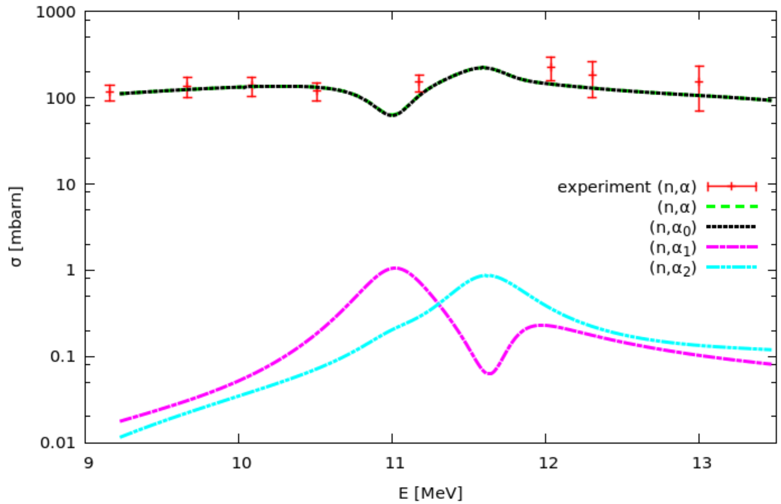
Excitation energy E_x of the compound nucleus defines energy scale:
channel representation for $R_{cc'}$, $S_{cc'}$, $T_{cc'}$, $V_{cc'}$

	$n+^{16}O$	$\alpha+^{13}C$	$p+^{16}N$	$d+^{15}N$
$n+^{16}O$	**elastic inelastic**			
$\alpha+^{13}C$		**elastic inelastic**		
$p+^{16}N$			**elastic inelastic**	
$d+^{15}N$				**elastic inelastic**

Fit capabilities for following experimental observables:

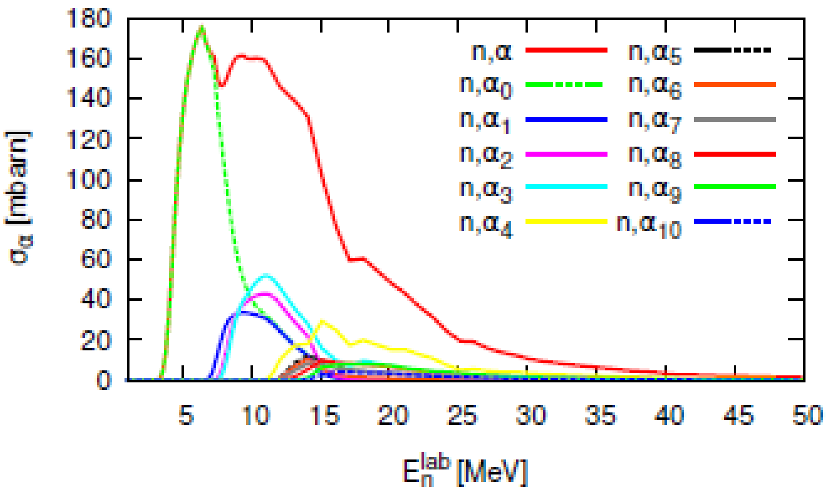
- angle integrated data
- angle differential data in cm- and lab-frame
- excitation functions in cm- and lab-frame
- analyzing power and vector polarization in cm- and lab-frame

Determining the best R-Matrix
How to deal with unknown $^{16}O(n,\alpha_i)$

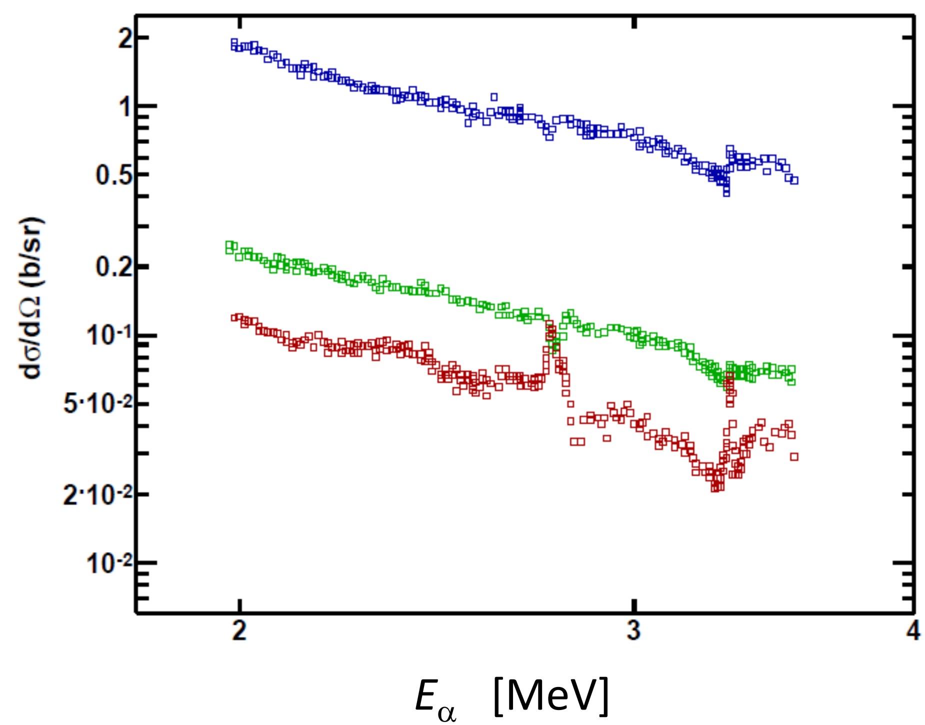


Additional Information on $^{16}O(n,\alpha_0)^{13}C$

- Inverse reaction $^{13}C(\alpha_0,n)^{16}O$
- Elastic scattering $^{13}C(\alpha_0,\alpha_0)^{13}C$



Excitation functions $^{13}C(\alpha,\alpha)$



Evaluation of Nuclear Data:
Current Status in Resonance Regime

Phenomenological R-matrix analyses $\{E_\lambda, \gamma_\lambda{}^c, c=a,\ldots,z\}$

M - finite number of poles
O - background poles introduced, mimic bulk interaction
D - partial wave identification may be ambiguous
E - not all resonances are included
L - frequently matching radius is optimized and channel-dependent

Codes:
EDA: unitary approach
SAMMY, REFIT and AZURE: use of Reich-Moore parametrisation

Covariance Matrix: limited to parameter uncertainties

$$\alpha = \frac{\partial^2 \chi^2}{\partial p_i \partial p_j} \quad ; \quad \langle \Delta\sigma(E)\Delta\sigma(E')\rangle = \sum_i \sum_j \frac{\partial\sigma(E)}{\partial p_i} \left(\alpha^{-1}\right)_{i,j} \frac{\partial\sigma(E')}{\partial p_j}$$

Problems: non-linearity of $\vec{\sigma}(E) = \vec{M}(\vec{p})$

Assumption: perfect model

Unified Evaluation Procedure

Intermediate energies: Statistical model calculations (GNASH, EMPIRE, TALYS)
optical potentials, level densities, precompoud factors, fission barrier, …

Resonance regime: R-matrix (SAMMY, REFIT, CONRAD, …; EDA,AZURE,AMUR,..)
pole and widths parameter, matching radius, …

R-matrix
Statistical model
Coupled-channel calc
Preequilibrium model
fission model
….

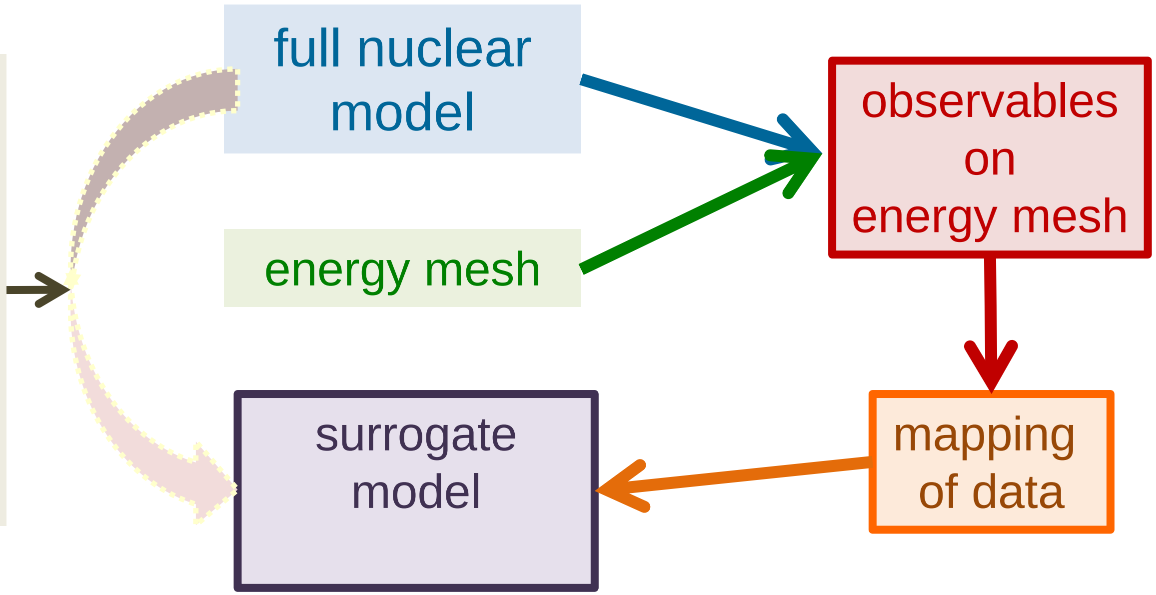
→

Observables
cross sections (integral,differential),
spectra, fission yields, …

A common evaluation must be on the basis of observables

Surrogate Model:
observables as model parameters

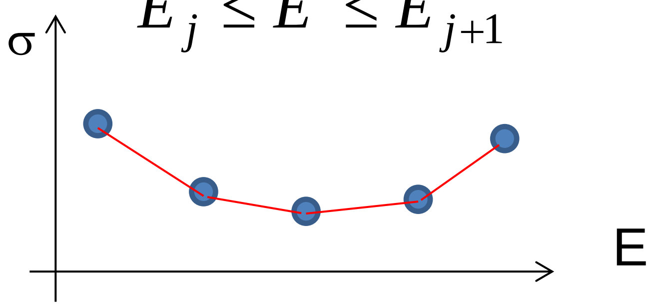
Main properties of nuclear model are transferred
- dominating eigenvalues
- summation properties



Linear mapping relation

$$E_j \le E' \le E_{j+1}$$

$$\sigma^{\mathrm{surr}}(E') = \left(\frac{\mathrm{E}_{j+1} - E'}{\mathrm{E}_{j+1} - E_j}\right)\sigma_j^{\mathrm{mod}} + \left(\frac{E' - \mathrm{E}_j}{\mathrm{E}_{j+1} - E_j}\right)\sigma_{j+1}^{\mathrm{mod}}$$



value of observable at mesh point

surrogate model

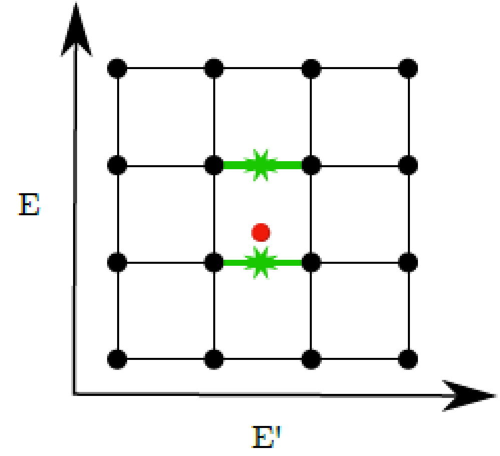
Surrogate Model:

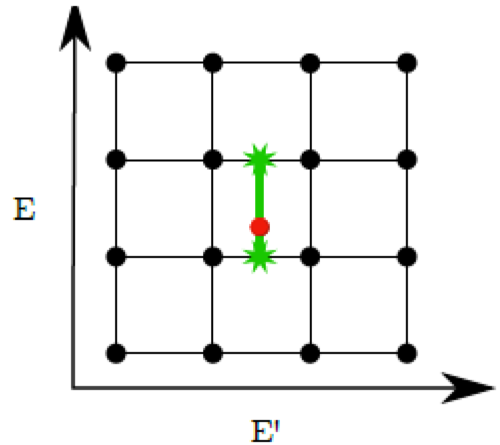
Representation of Angular and Energy Differential Data

Differential Data:

- angle differential data $\vec{\sigma}(E,\Omega)$
- energy differential data $\vec{\sigma}(E,E')$

bilinear interpolation





Properties of linear and bilinear interpolation

- simple,scarce matrices for mapping
- sums are conserved in each inter-polated point
- negative cross sections cannot occur

Price to pay

dense mesh is required for proper presentation

Unified Evaluation Procedure
Required Steps

Step 1: best TALYS representation in the statistical model regime
Step 2: use boundary values at transition point and search for best R-matrix representation.

Step 3: define surrogate model (energy model mesh)

Step 4: (a) Generate prior covariance for statistical model regime
(b) Generate prior covariance for R-matrix regime
Step 5: generate combined prior covariance matrix $\mathbf{A}_0$

Step 6: determine covariance matrix **B** for experiments

Step 7: determine covariance matrix $\mathbf{K}_0$ for model defects

Step 8: perform Bayesian update and evaluate $\vec{\sigma}_1, \vec{\varepsilon}_1, \vec{\sigma}_{true} = \vec{\sigma}_1 + \vec{\varepsilon}_1$

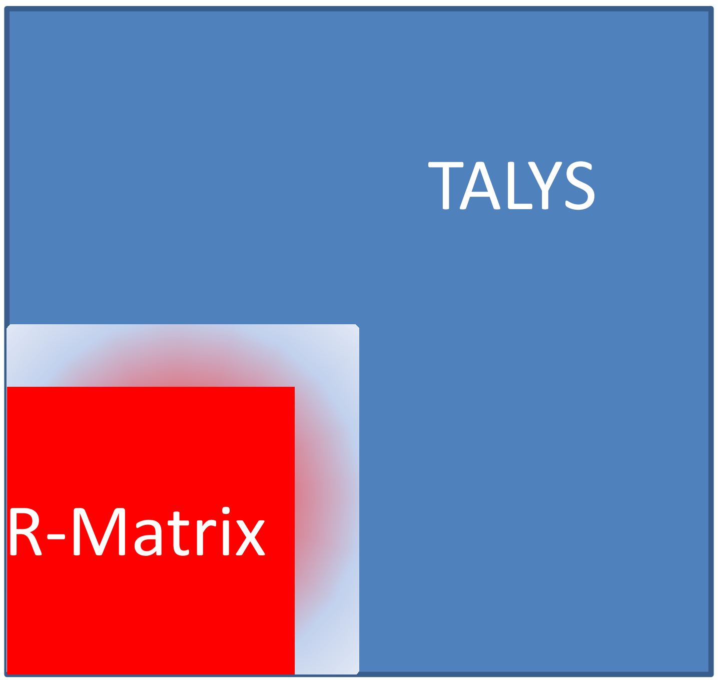
A_1, K_1, U_1

Unified Evaluation Procedure
The Combined Prior Covariance Matrix

Step 5: Combined prior covariance matrix

$$A_0(E,E') = f(E,E')A_0^{RMat}(E,E') + \left[1 - f(E,E')\right]A_0^{TALYS}(E,E')$$

$A_0 =$



The properties between the statistical model regime are partially transferred via the combined covariance matrix A_0

The evaluation is by definition continuous with a smooth transition region.

Unified Evaluation Procedure:

Statistically consistent Treatment of Model Defects

Standard Evaluation:

$$\vec{\sigma}_{\text{exp}} = \vec{\sigma}_{\text{mod}} + \vec{\varepsilon}_{\text{exp}}$$

Experiment vector   Model vector   Uncertainty vector of experiment

$$\vec{\sigma}_{\text{exp}} = \vec{\sigma}_{\text{mod}} + \vec{\varepsilon}_{\text{mod}} + \vec{\varepsilon}_{\text{exp}}$$

Extended Evaluation:

Model defect

PhD thesis of Georg Schnabel (TU Wien, June 2015)

Unified Evaluation Procedure

Accounting for Model Defects

Model Defects: account for deficiencies of the model
functional form not known → described by Gaussian processes

Assumption: $\langle \vec{\varepsilon}_{\text{mod}} \rangle = 0 \,, \qquad \langle \varepsilon_{\text{mod}}(E)\,\varepsilon_{\text{mod}}(E') \rangle = K_0$

The assumed covariance matrix for model defects can be composed of different terms.

Model Defects in the Unified Evaluation Procedure

$$\langle \vec{\varepsilon}_{\text{mod}} \rangle = 0 \,,\; K_0 = \langle \varepsilon_{\text{mod}}(E)\,\varepsilon_{\text{mod}}(E') \rangle = K_0^{\text{StatMod}} + K_0^{\text{Resonances}} + K_0^{\text{AngDistr}} + \cdots$$

New term suitable for model defects in resonances
Refer to presentation by B. Raab on Friday morning

Unified Evaluation Procedure

Performing Bayesian Update

Surrogate Model: $\vec{\sigma}_{exp} = S_{exp}\vec{\sigma}_{mod} + T_{exp}\vec{\varepsilon}_{mod} + \vec{\varepsilon}_{exp}$

Bayesian Update in linearized form → GLS

$$\vec{\sigma}_1 = \vec{\sigma}_0 + A_0 S_{exp}^T X\vec{\alpha} \qquad A_1 = A_0 - A_0 S_{exp}^T X S_{exp} A_0$$

$$\vec{\varepsilon}_1 = K_0 T_{exp}^T X\vec{\alpha} \qquad K_1 = K_0 - K_0 T_{exp}^T X T_{exp} K_0$$

change to standard GLS

with

$$\vec{\alpha} = \left(\vec{\sigma}_{exp} - S_{exp}\vec{\sigma}_0\right) \qquad X = \left(S_{exp}A_0 S_{exp}^T + T_{exp}K_0 T_{exp}^T + B\right)^{-1}$$

Data for evaluated File:

$$\vec{\sigma}_{true} = \vec{\sigma}_1 + \vec{\varepsilon}_1 \qquad C_0 = S_{comb}A_0 S_{exp}^T + K_0 T_{exp}^T$$

$$U_1 = U_0 - C_0 X C_0^T \qquad U_0 = S_{comb}A_0 S_{comb}^T + K_0$$

Performing the Evaluation:
Generating an ENDF File

The ENDF-File generated is based on

a) R-matrix fit with background potential and pole terms at
1 MeV < E < 13 MeV
MF=3: MT=1 (total), 2 (elastic), 3 (non-elastic), 51-55 (n,n'_i),800-805 (n,a_i)
MT=103 (n,p), MT=104 (n,d), MT=105 (n,t)
MF=4: MT=2, MT=800 isotropic in c.m.

b) Statistical model calculations by TALYS with optimized optical potentials and level densities (ENDF File Option)

The file is generated from modified TALYS output via the code TEFAL (A. Koning), hence the file are of similar structure as those in the TENDL Library.

The developed codes system is successfully tested on integral and differential data. However, the demonstration on n-^{16}O experimental data was limited so far on integral data.

Summary and Outlook

Hybrid R-matrix approach developed for light nuclear systems

Unified evaluation procedure formulated

Corrsponding numerical tools developed
code GECCCOS, code GENEUS

First application to n+^{16}O performed

Open Problems

- Treatment of breakup reactions and multi-particle channels
- Unitary treatment of capture reactions
- Implementation of modified General Least Square Method

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Thank you for your attention