

Tools for Benchmarking of
Spallation Models
&
-First results

M. U. Khandaker
IAEA

OBJECTIVES of the “Benchmark of Spallation Models”

- **To assess the prediction capabilities of the spallation models**
used or that could be used in the future in high-energy transport codes.
- **To understand the reason for the success or deficiency of the models**
in the different mass and energy regions or for the different exit channels
- **To reach a consensus, if possible,**
on some of the physics ingredients that should be used in the models.

Way to achieve the goals/meet the targets

- ✓ Selection of an agreed set of experimental data for benchmarking of spallation models (**Done in TRIESTE**)
- ✓ Collections of spallation models calculations corresponding to exp. ones
&
Develop tools to do a comparative study
- **Analyze the results to meet the objectives**

Status of Participants/Codes

Codes	Neutron	neutron multi.	Lcp	Pion	Residue	Excfn	Add. Info.	Ingredients
CEM0303*	✓		✓	✓	✓	✓	✓	
CEM0302*	✓		✓	✓	✓	✓	✓	✓
PHITS-jam	✓	✓	✓	✓	✓	✓		✓
PHITS-bertini	✓	✓	✓	✓	✓	✓		
PHITS-jqmd		✓	✓		✓			✓
Cascade04	✓		✓	✓	✓	✓		✓
Isabel-smm*	✓	✓	✓	✓	✓		✓	
Isabel-gemini++*	✓	✓	✓	✓	✓		✓	
Geant4-binary	✓		✓	✓	✓	✓		✓
Geant4-bertini	✓		✓	✓	✓	✓		✓
Cascadeasf	✓							

* Data given for isotopic targets

List of Foreseen Calculations/Codes

Code	Participants
INCL4+ABLA	Participants : J Cugnon, A Boudard, A Kelic Affiliation : Liege University, CEA Saclay, GSI Darmstadt
INCL4+GEMINI	Participants: J Cugnon, A Boudard, R Charity Affiliation: Liege University, CEA Saclay, University of S Louis
INCL4+SMM	Participants: J Cugnon, A Boudard, A Botvina Affiliation: Liege University, CEA Saclay, Russian Academy of Science
ISABEL+ABLA	Participants: Y Yariv, A Kelic Affiliation: Soreq NRC, GSI-Darmstadt
FLUKA*	Participants: A Ferrari Affiliation: CERN

*** To be confirmed**

Additional information

?

- To understand the reason for success or deficiency
- Useful to analyze the results

P_Fe_1200_info		CEM03-02	CEM03-03	Isabel-gemini	Isabel-smm
Reaction σ , (mb)		739.8	739.8		
σ for Norm, (mb)		744.4	744.31	733.752	739.41
Characteristics remnant nucleus					
Before preeq	E*av (MeV)	169.1	169.1	68.64	68.20
	Zav	24.5	24.5	24.61	24.62
	Aav	51.6	51.6	52.80	52.81
	Lav	7.0	7.0		
	E*/A (MeV)	3.42		1.33	1.32
	P _R (MeV/c)	525.8			
Before de-excitation	E*av (MeV)	143.3	147.3		
	Zav	24.0	23.9		
	Aav	50.6	50.5		
	Lav	7.9	8.1		
	E*/A (MeV)	2.98			
	PR (MeV/c)	518.5			
Multiplicities					
	Neutron (Mn)	5.546	5.4976	1.98 (de-exct)	2.23 (de-exct)
	Proton (Mp)	4.543	4.4905	1.31 (de-exct)	1.028 (de-exct)
	Deuteron (Md)	1.264	1.2444	0.154 (de-exct)	0.105(de-exct)
	Tritium (Mt)	0.2627	0.2596	0.0333 (de-exct)	0.0311 (de-exct)
	Helium-3 (Mhe3)	0.2307	0.2266	0.0133 (de-exct)	0.0185 (de-exct)
	Alpha (Mhe4)	0.7548	0.7429	0.274	0.174

Steps of work

- ❑ Checking and/or making standard format of all data files
- ❑ Creating scripts and/or develop programs for plotting of
 - Double differential cross section
 - Neutron production
 - Light charged particle production
 - Pion production
 - Neutron multiplicity distribution
 - Residue production
 - Isotopic distribution
 - Excitation function
 - Independent production of nuclides
 - Cumulative production of nuclides

Checking and/or making standard format of all data files

- For a benchmark work, we need to handle a large volume of data files by some relevant tools
- consequently, all data files should be in similar format

However,

-- NOT a difficult task,
but time consuming & (boring!!!!)

1. Example for data file names

Codes	Given file names
CEM0302	p_ Au197_ 1200_ ddxshe3_ cem03_ 02
CEM0303	p_ Au197_ 1200_ ddxsHe3_ cem0303
PHITS-jam	p_ Au_ 1200_ ddxs3he_ phits(JAM)
PHITS-bertini	p_ Au_ 1200_ ddxs3he_ phits(Bertini)
PHITS-jqmd	p_ Au_ 1200_ ddxs3he_ phits(JQMD)
Cascade04	p_ Au_ 1200_ ddxs_ He3_ cascade04
Isabel-smm	p_ au197_ 1200_ ddxshe3_ isabel-smm
Isabel-gemini	p_ au197_ 1200_ ddxsHe3_ isabel-gemini++
Geant4-binary	p_ Au_ 1200_ ddxshe3_ g4bic
Geant4-bertini	p_ Au_ 1200_ ddxshe3_ g4bert
Experiment data	p_ Au_ 1200_ ddxshe3_ budzanowski

2. Example: situation for the angular grid

File name	Participants	Angular grid
P_Fe_1200_ddxsn	leray et al. (exp.)	0, 10, 25, 40, 55, 85, 100, 115, 130, 145, 160 (Expected angular grid)
	CEM0302	2, 10, 25, 40, 55, 85, 100, 115, 130, 145, 160
	CEM0303	0, 10, 25, 40, 55, 85, 100, 115, 130, 145, 160
	PHITS-jam	0, 10, 25, 40, 55, 75, 85, 100, 115, 130, 145, 160
	PHITS-bertini	0, 10, 25, 40, 55, 75, 85, 100, 115, 130, 145, 160
	Cascade-asf	No data
	Cascade04	0, 10, 25, 40, 55, 60, 85, 100, 115, 120, 130, 145, 150, 160
	Isabel-smm	0, 10, 25, 40, 55, 85, 100, 115, 130, 145, 160
	Geant4-binary	2, 6, 10, 15, 20, 25, 30.5, 35, 40, 47.5, 55, 60, 65, 71.5, 77.5, 85, 92.5, 100, 107.5, 115, 122.5, 130, 137.5, 146, 158.5, 167.5, 175
	Geant4-bertini	2, 6, 10, 15, 20, 25, 30.5, 35, 40, 47.5, 55, 60, 65, 71.5, 77.5, 85, 92.5, 100, 107.5, 115, 122.5, 130, 137.5, 146, 158.5, 167.5, 175

Tools for data handling

Plotting software : **gnuplot**
Language used : **Fortran, Perl**
System : **Unix**

Creation of Scripts/ Developed programs

Several scripts have been created for plotting of

Experimental data

versus

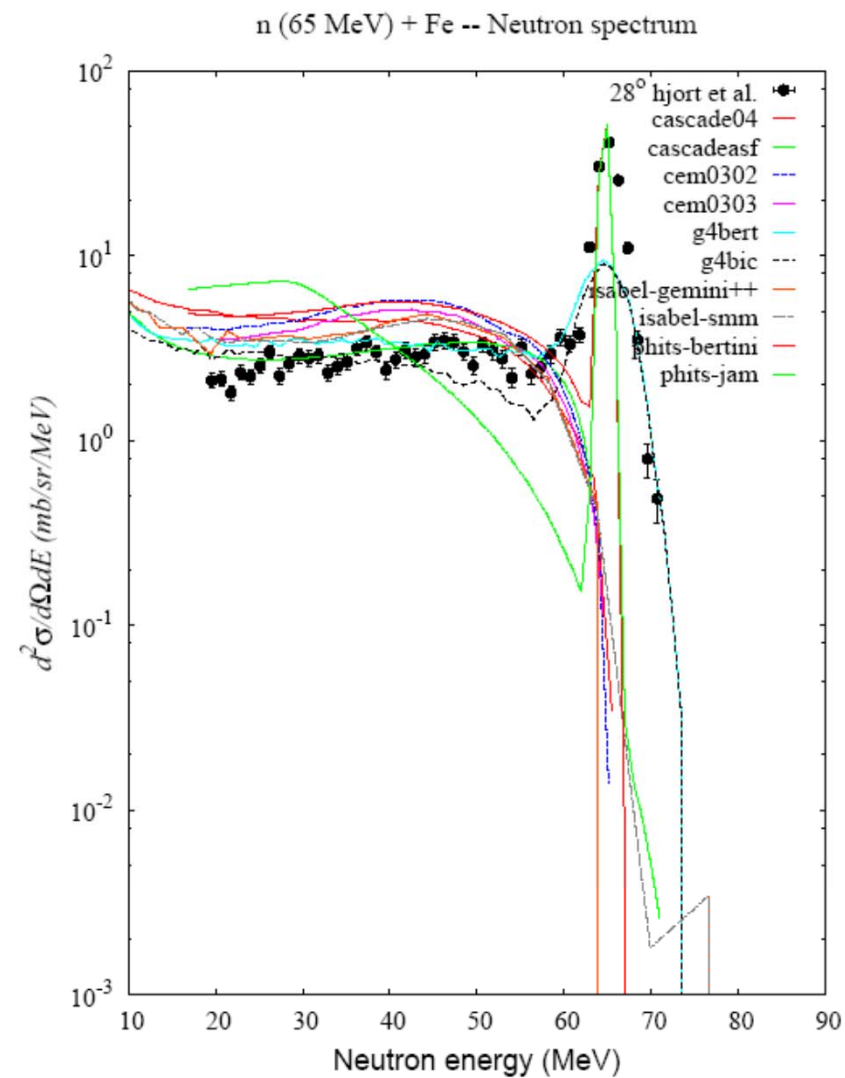
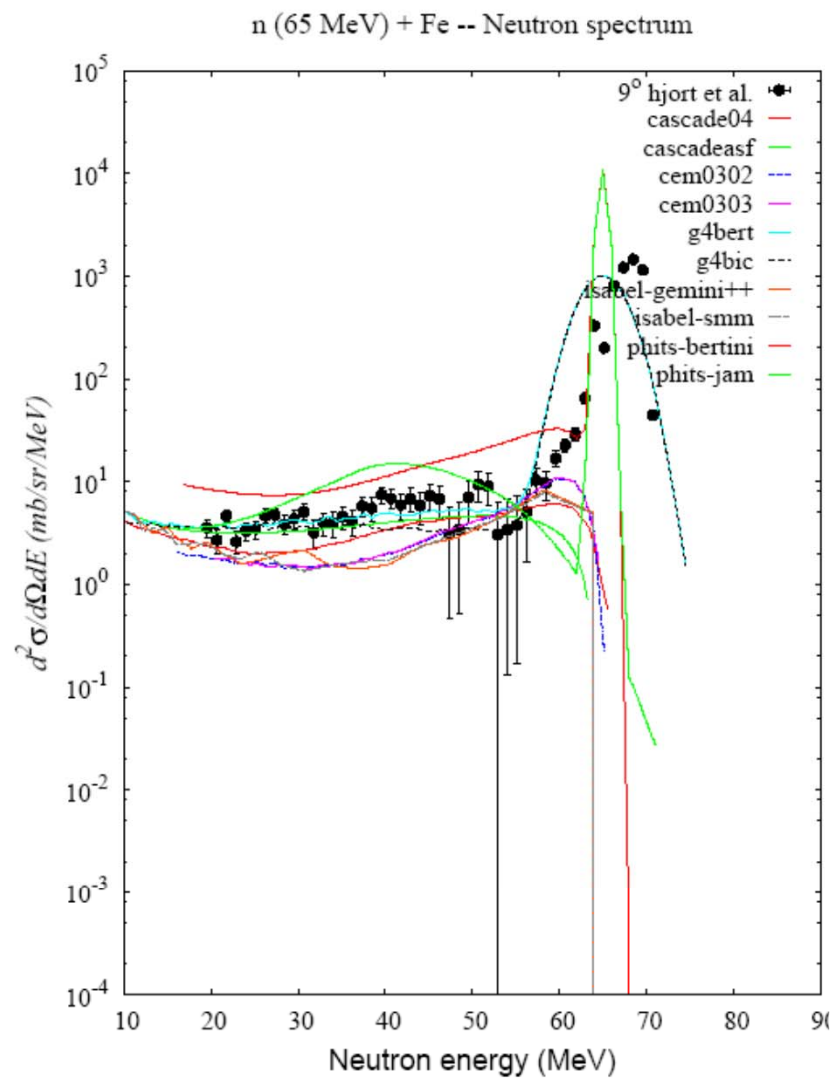
Any combination of model calculations

- Examples → Exp. data vs. all angle / model #1
→ Exp. data vs. all angle / model #1, #2, #3,..
→ Exp. data vs. one angle / model #1
→ Exp. data vs. one angle / model #1, #2, #3,..

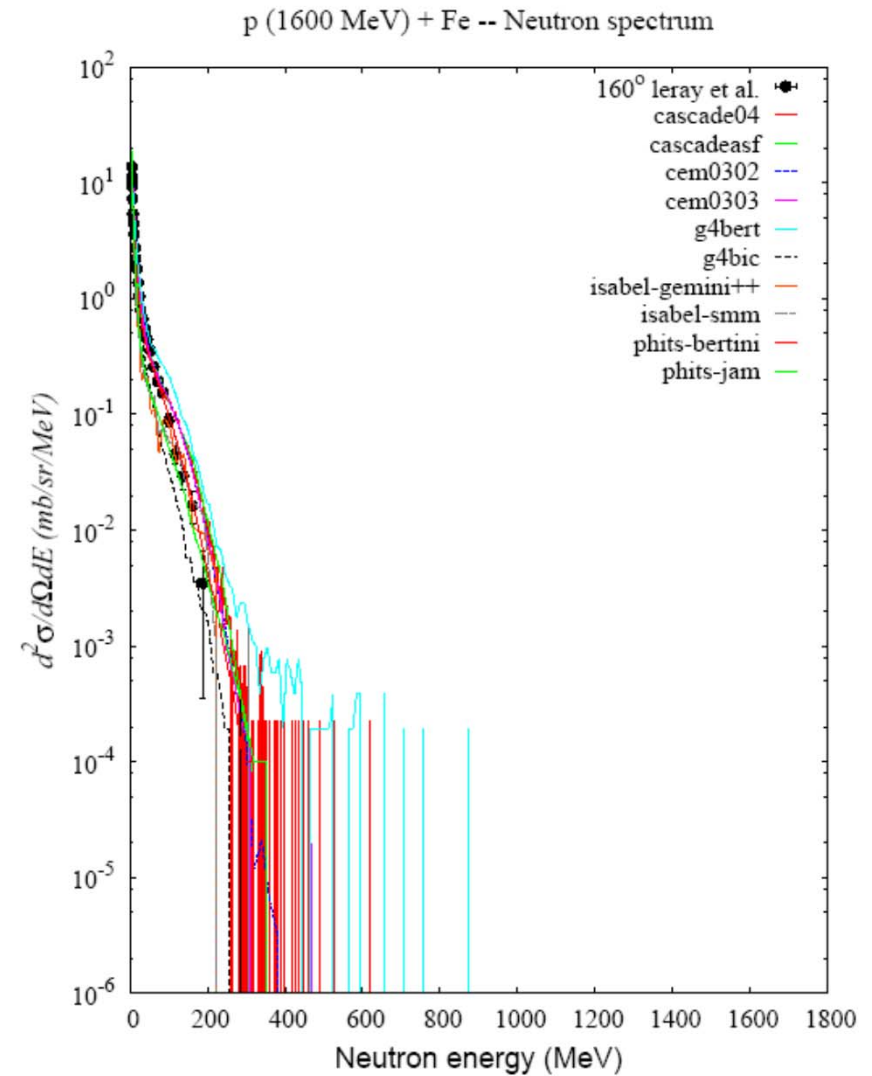
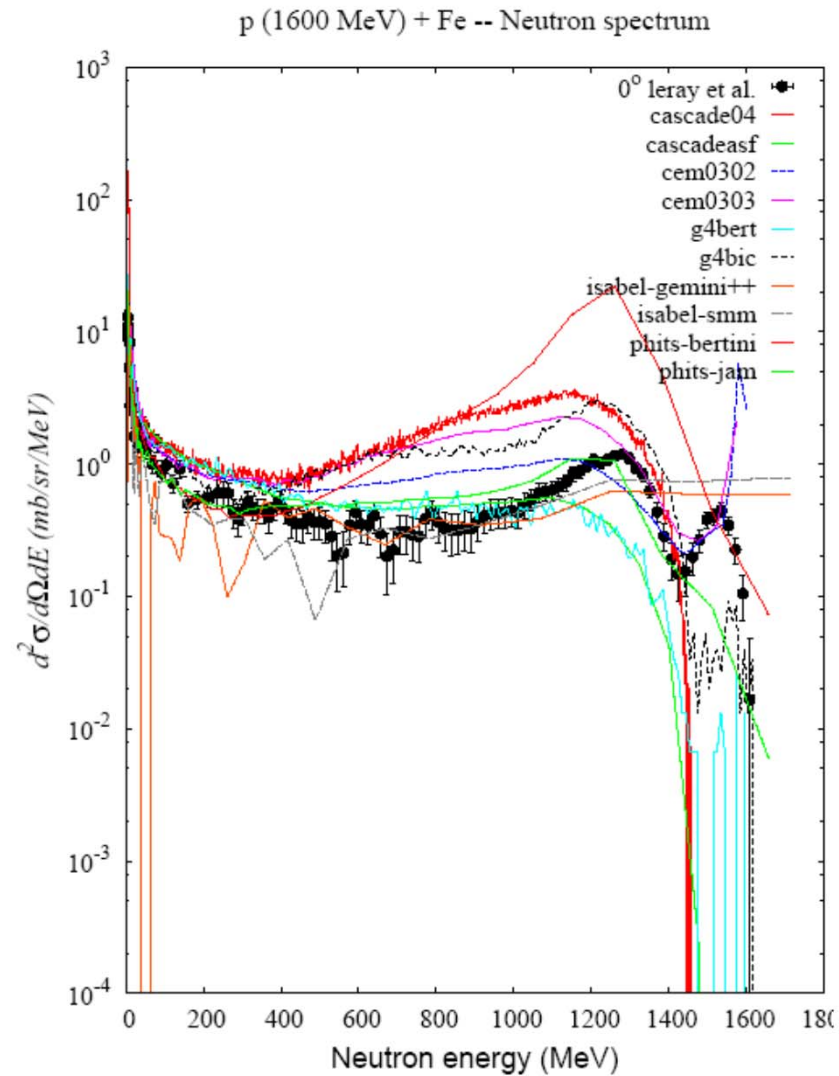
1. Neutron Spectrum

Examples

Neutron spectrum with low energy projectile



Neutron spectrum with high energy projectile



**For neutron production- as a test case,
we placed the data and figures of all
calculations in the Spallation Web site**

<http://www-nds.iaea.org/spallations/>

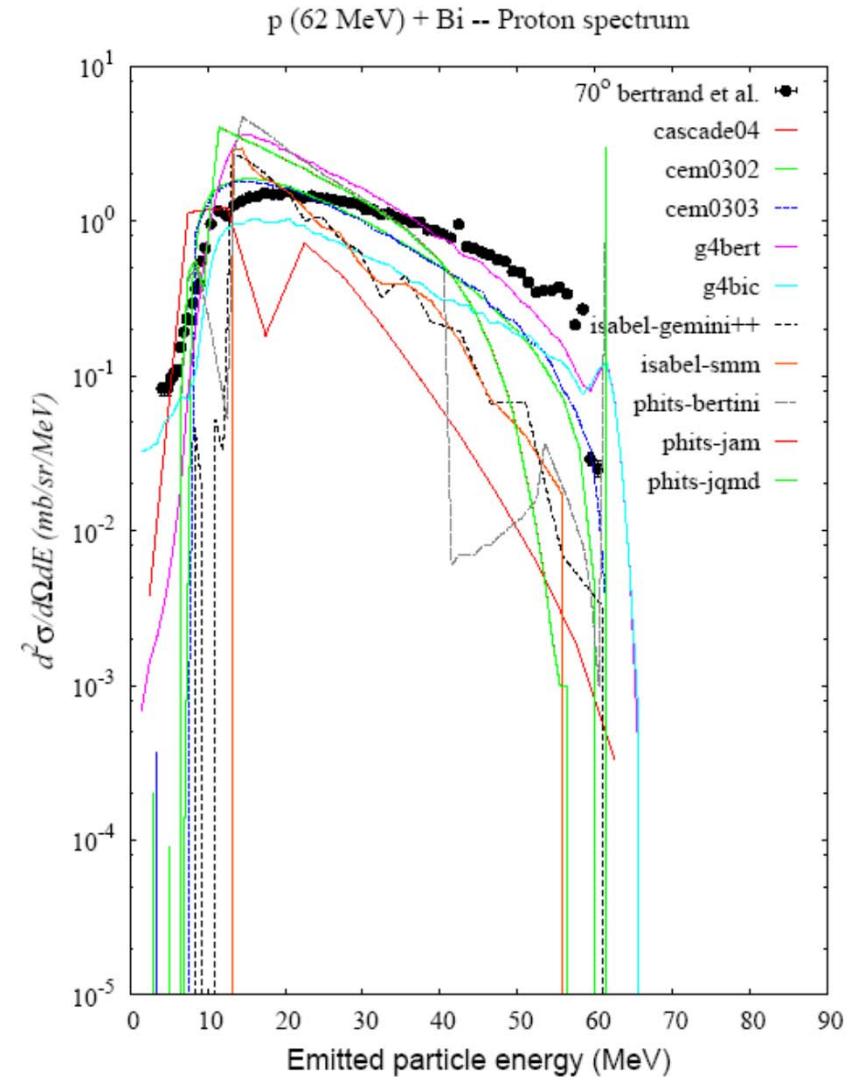
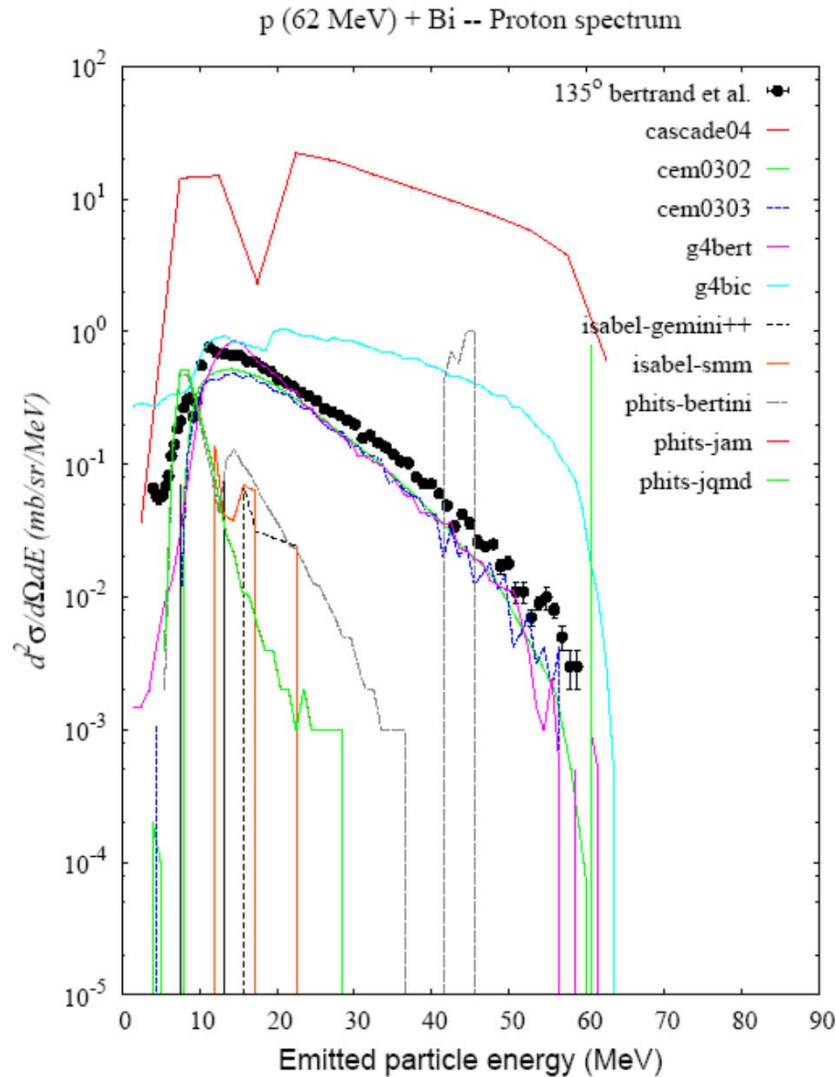
2. Light Charged Particle production

Examples

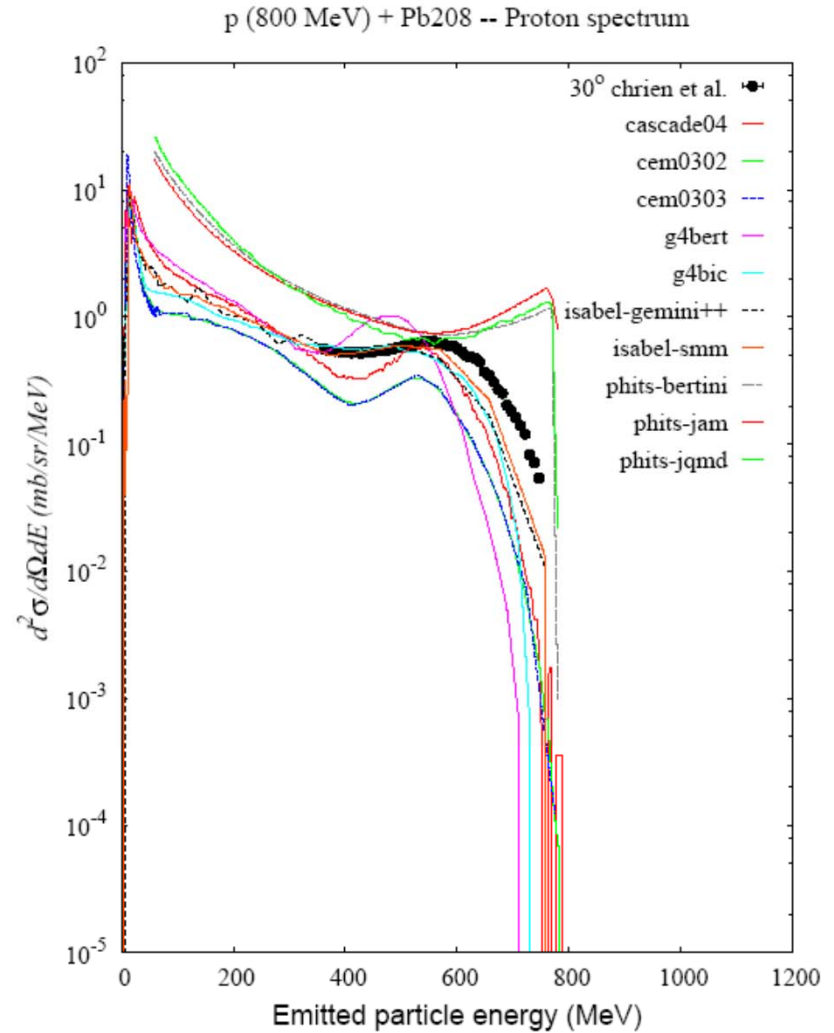
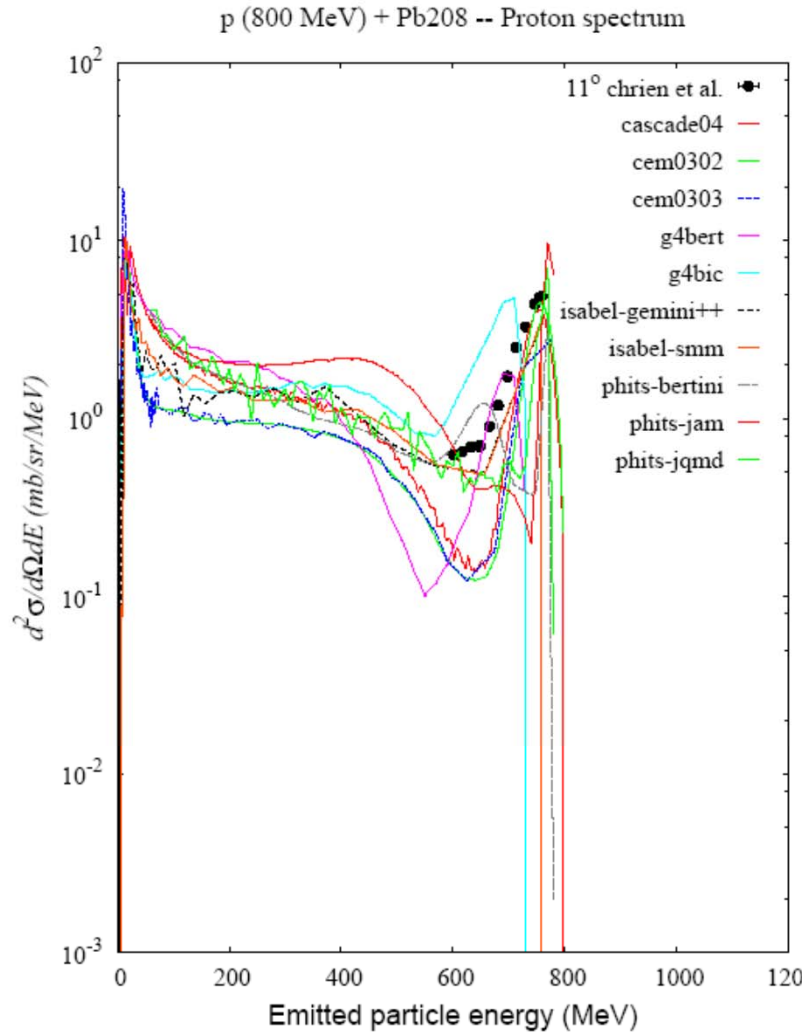
Proton Spectrum with low energy projectile

Overestimated

Underestimated

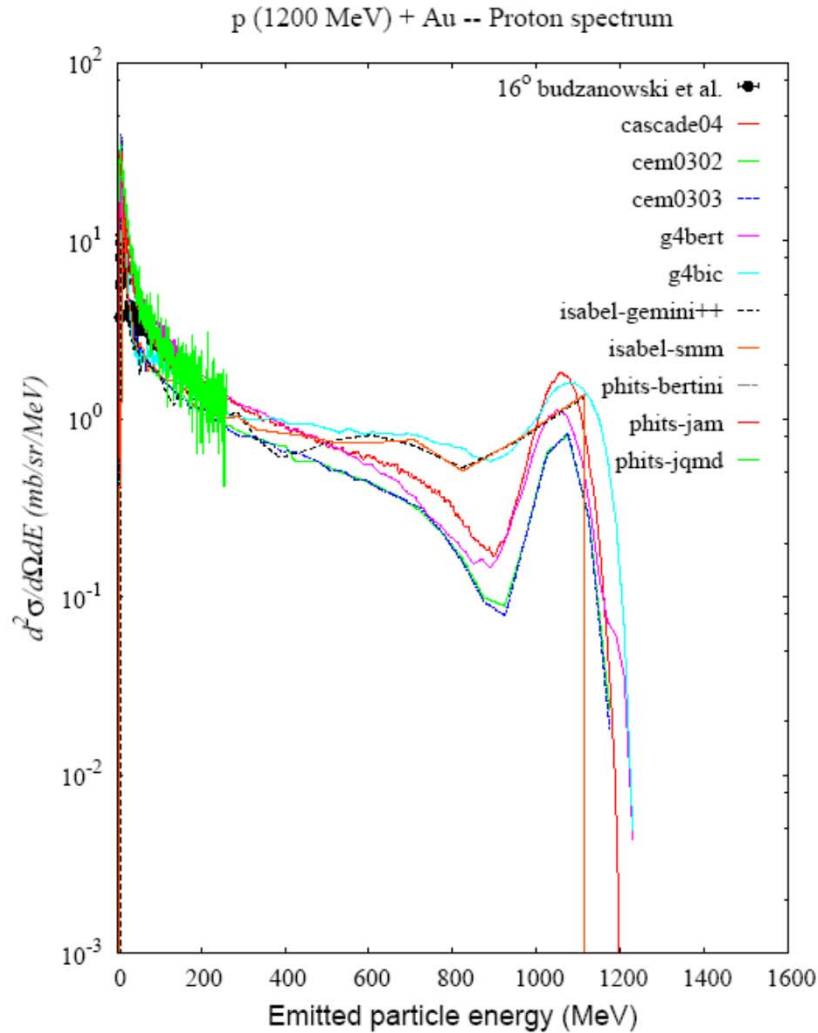


Proton Spectrum with high energy projectile

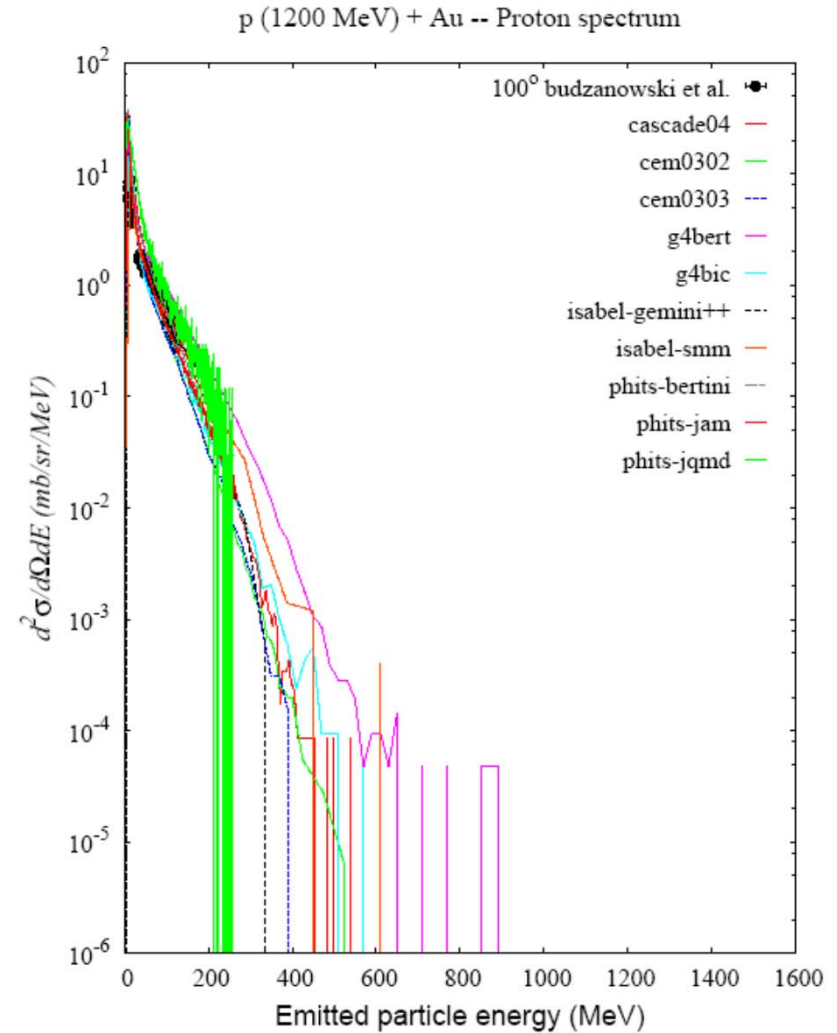


Proton Spectrum with high energy projectile

Forward angle



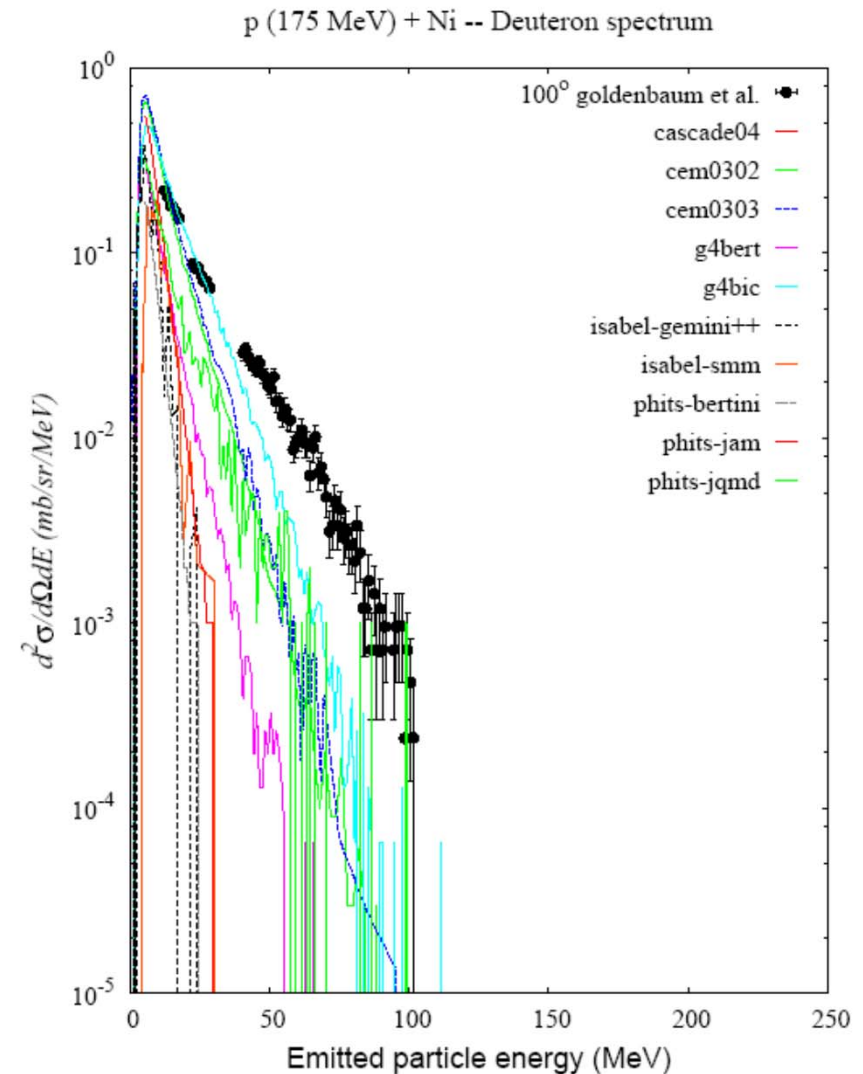
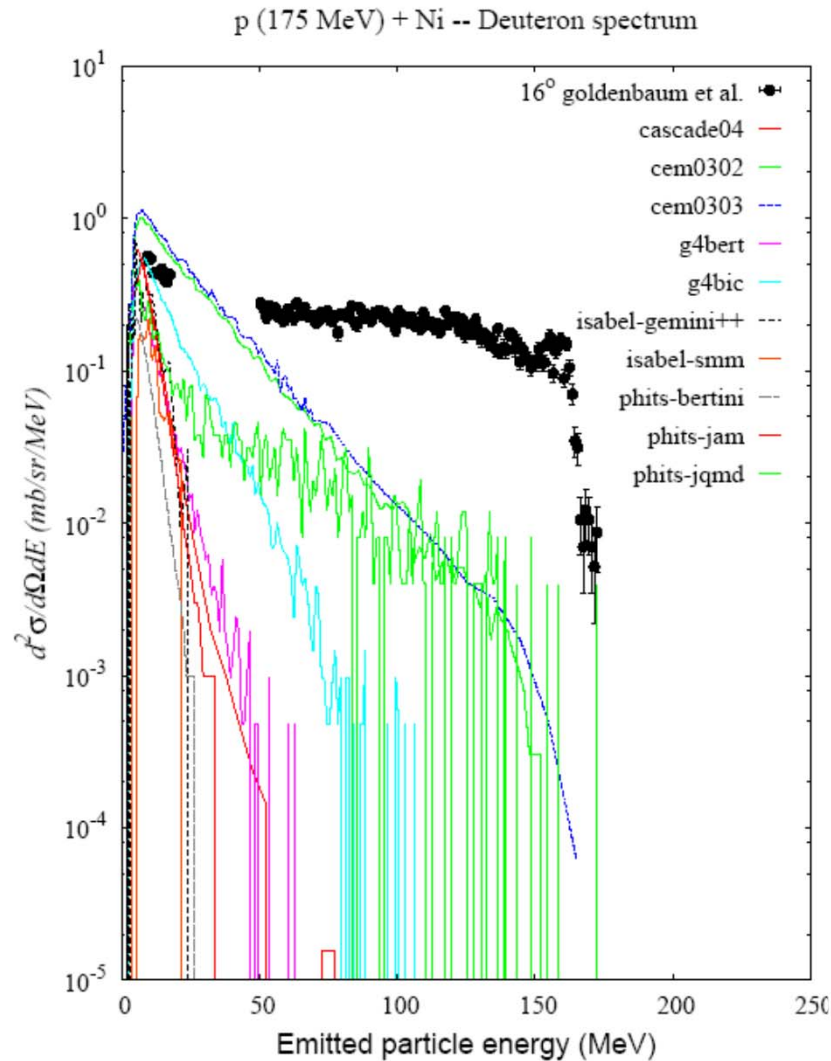
Backward angle



Deuteron Spectrum with medium energy projectile

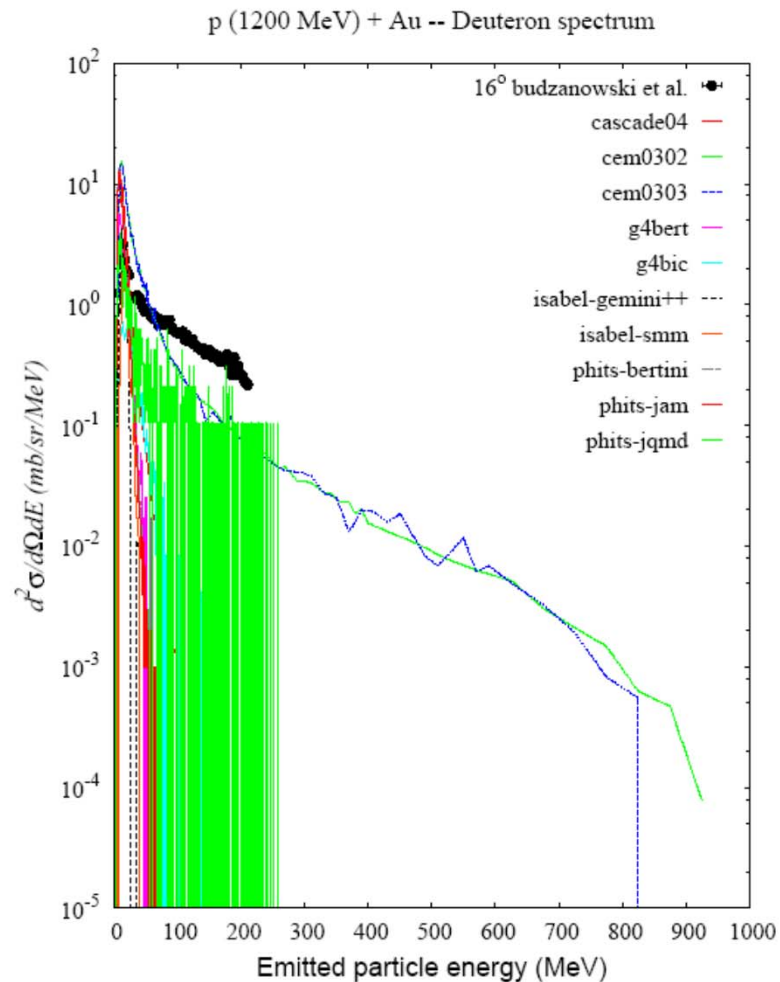
Forward angle

Backward angle

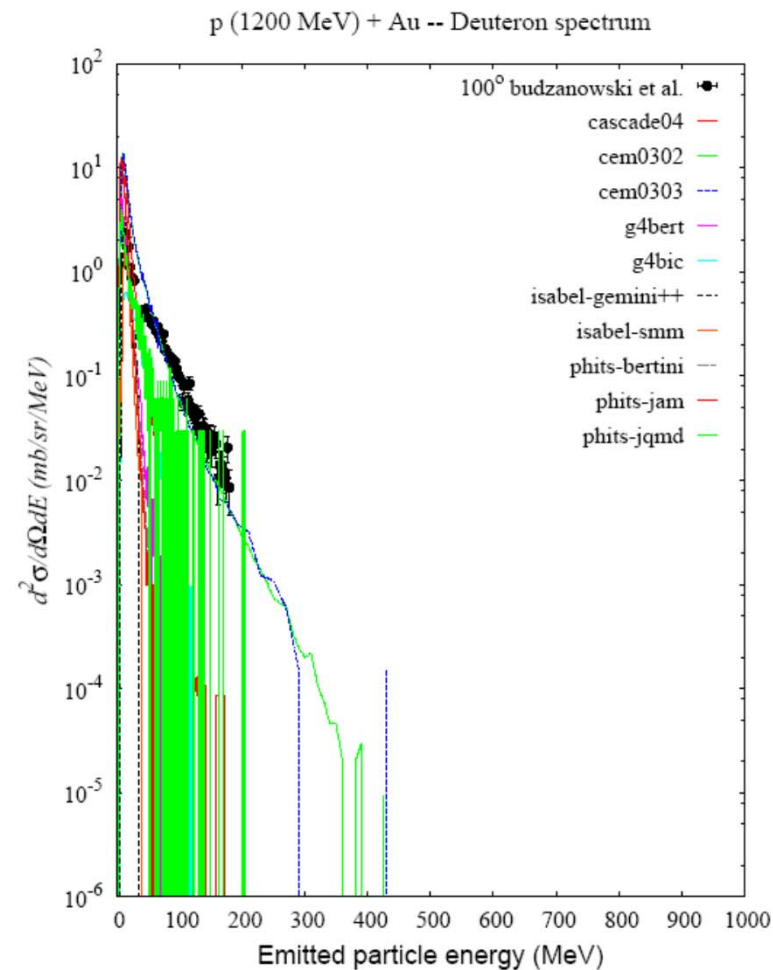


Deuteron Spectrum with high energy projectile

Forward angle



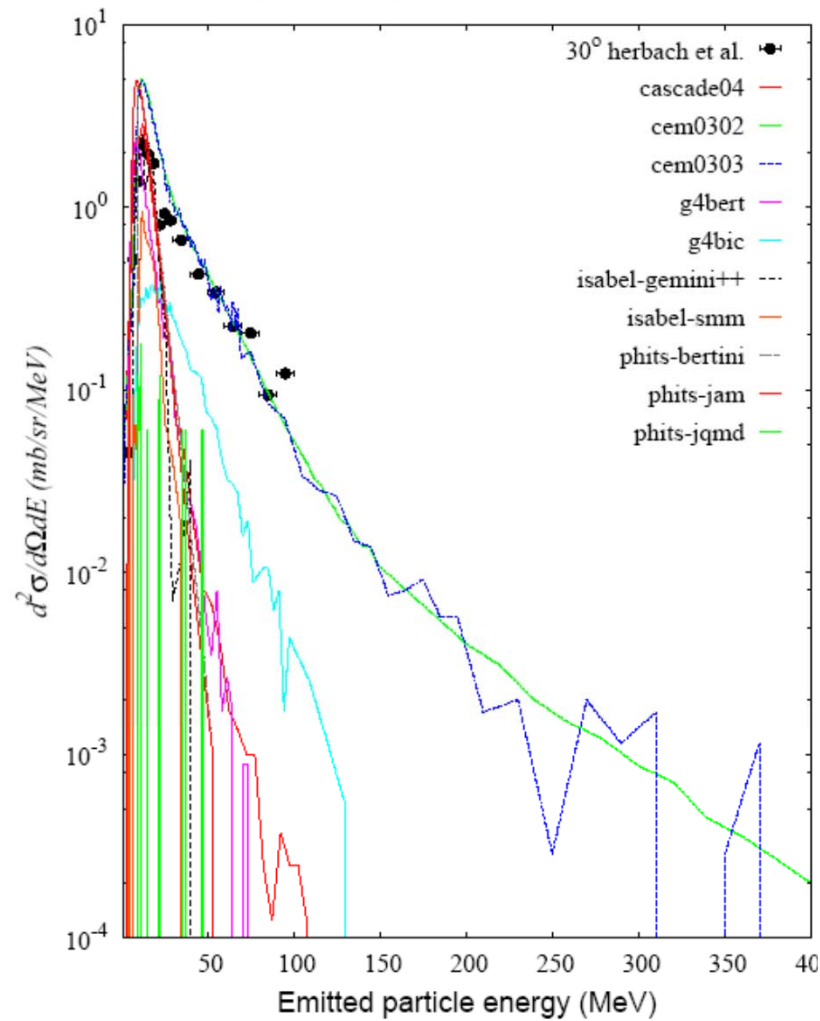
Backward angle



Tritium Spectrum with high energy projectile

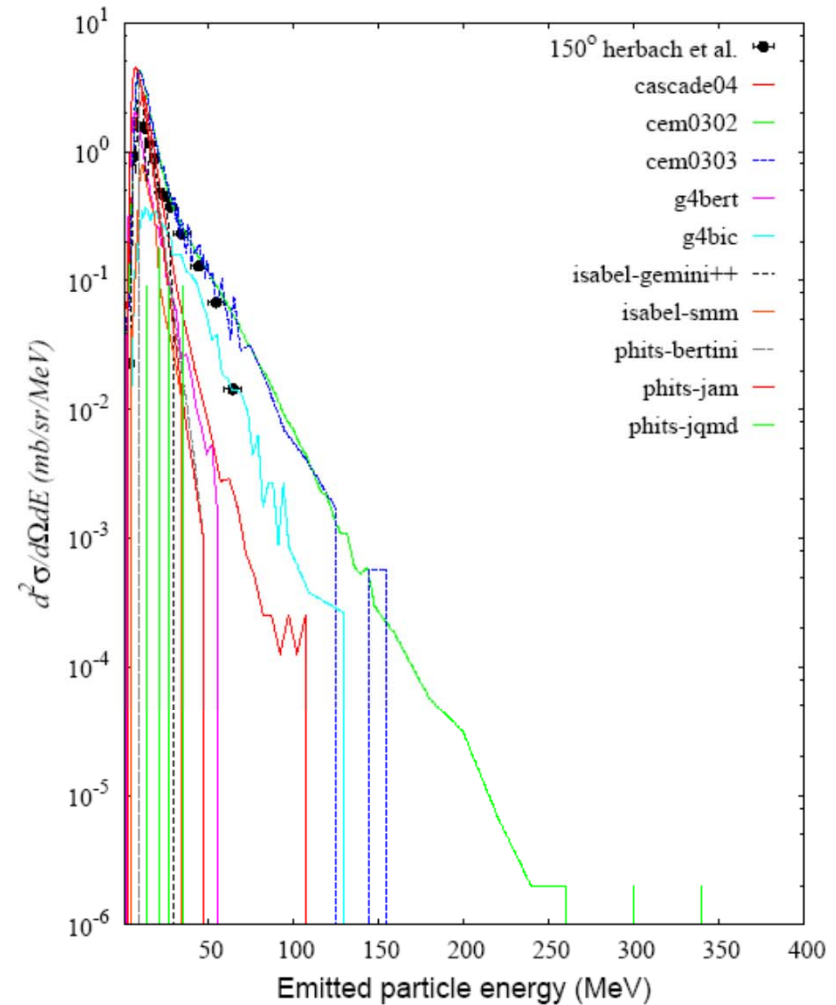
Forward angle

p (1200 MeV) + Ta -- Tritium spectrum



Backward angle

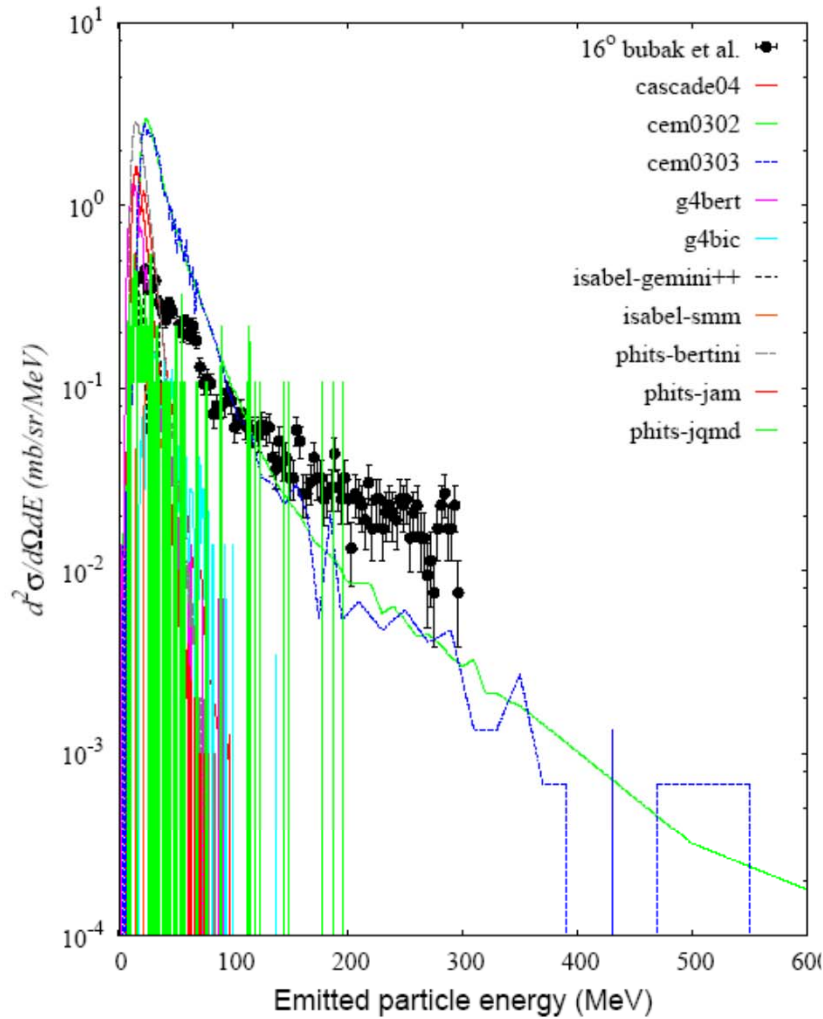
p (1200 MeV) + Ta -- Tritium spectrum



Helium-3 Spectrum with high energy projectile

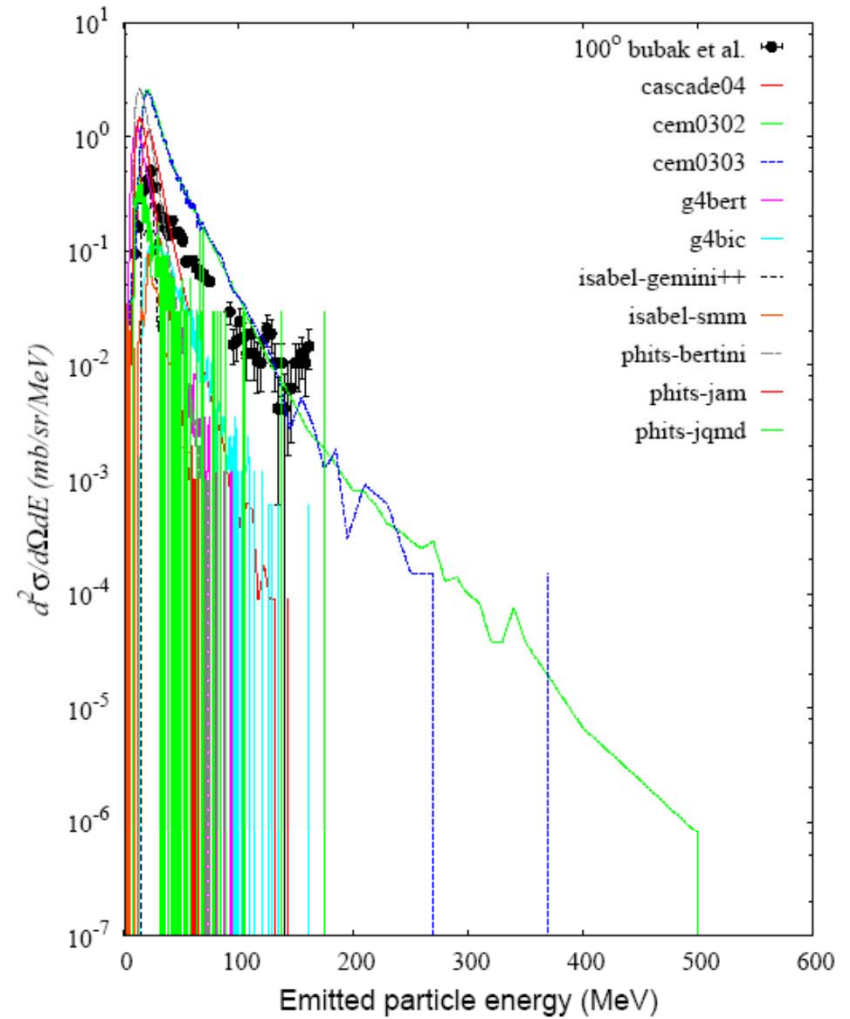
Forward angle

p (2500 MeV) + Au -- Helium-3 spectrum



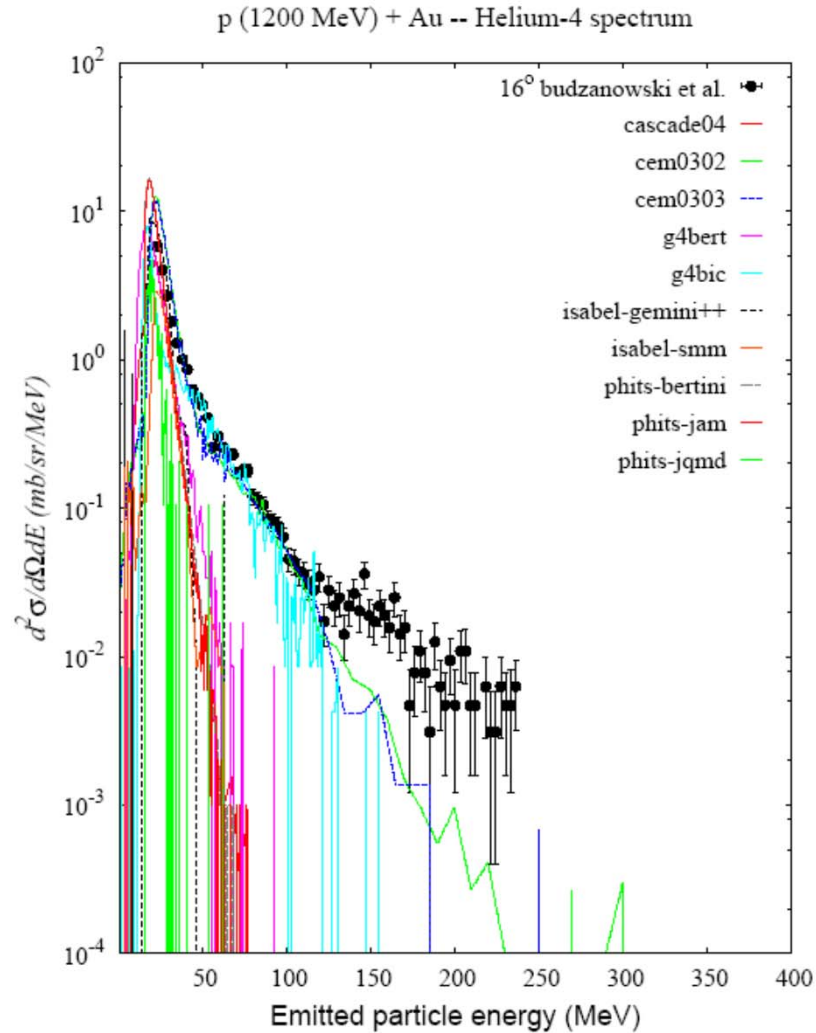
Backward angle

p (2500 MeV) + Au -- Helium-3 spectrum

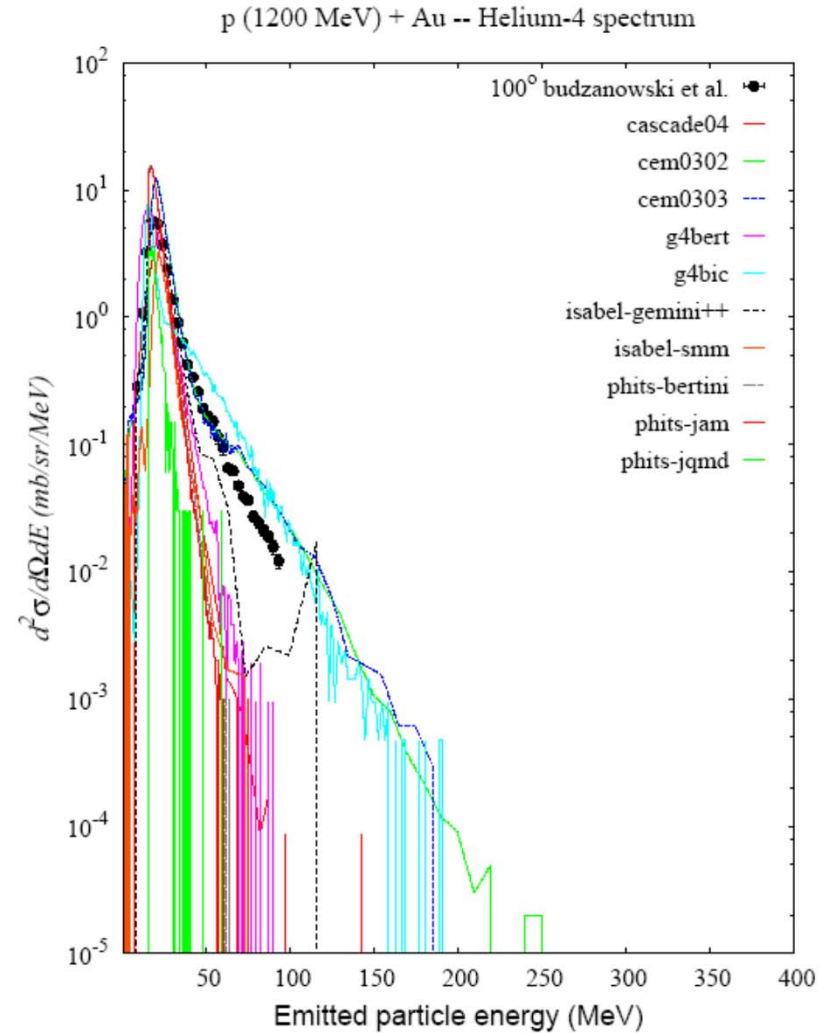


Alpha Spectrum with high energy projectile

Forward angle

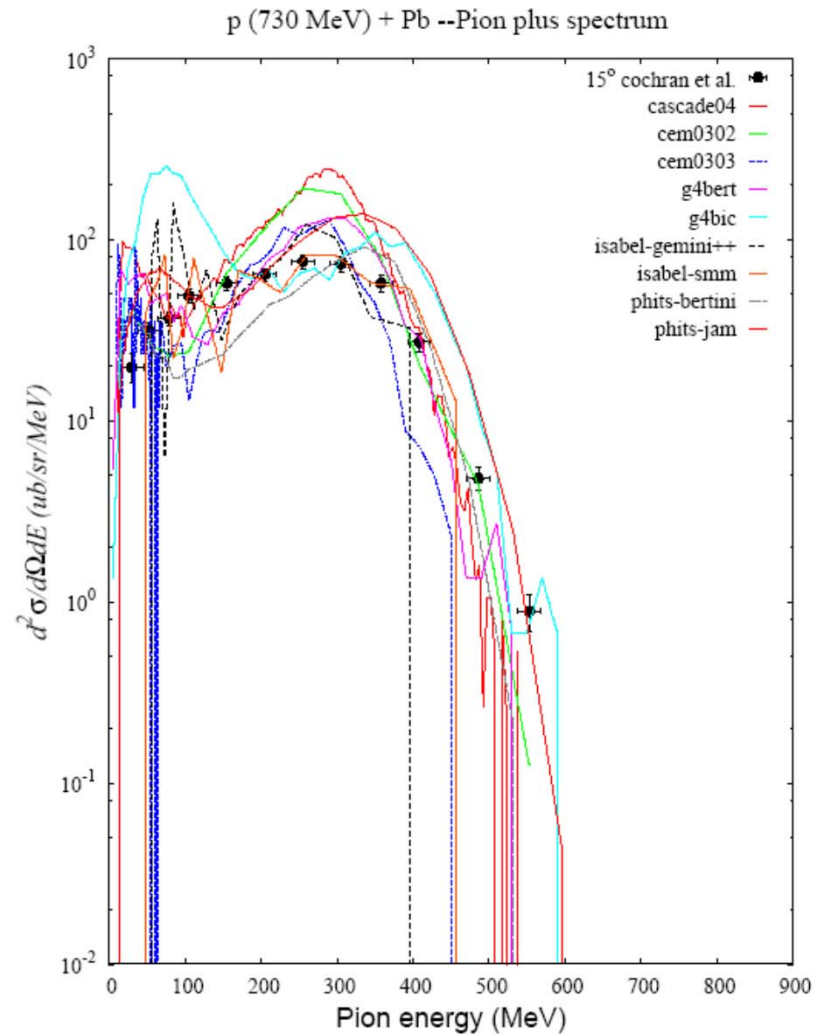


Backward angle

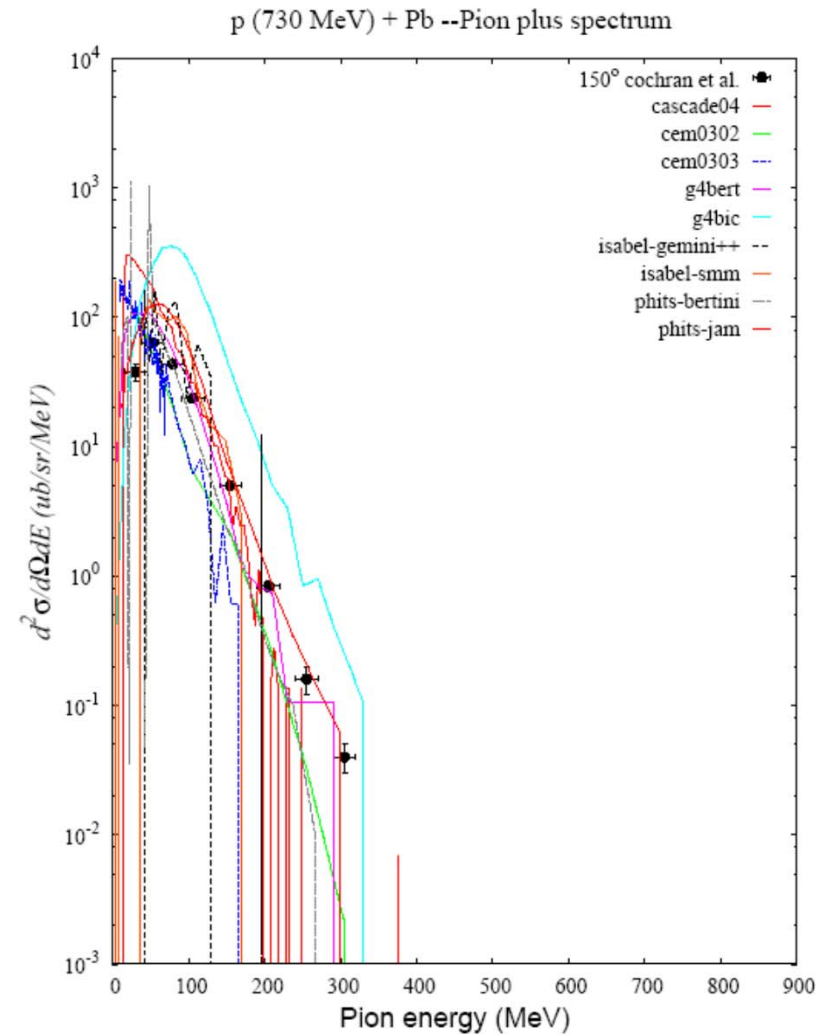


Pion plus production

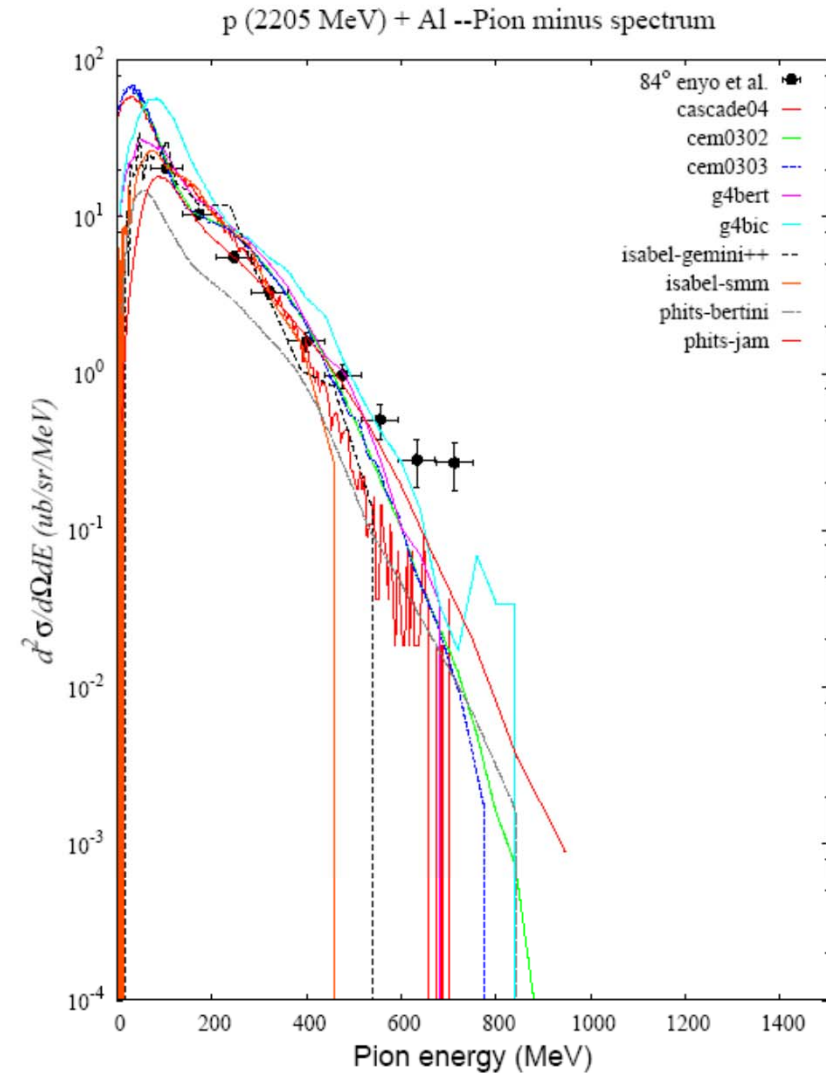
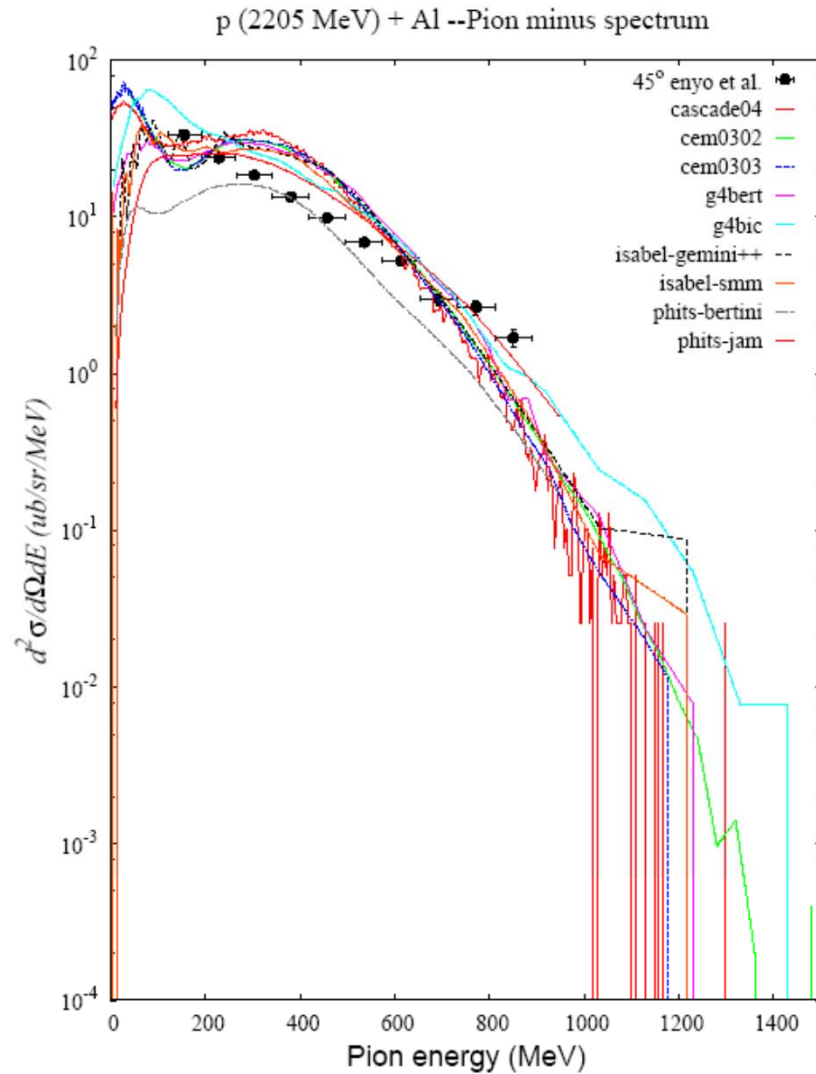
Forward angle



Backward angle

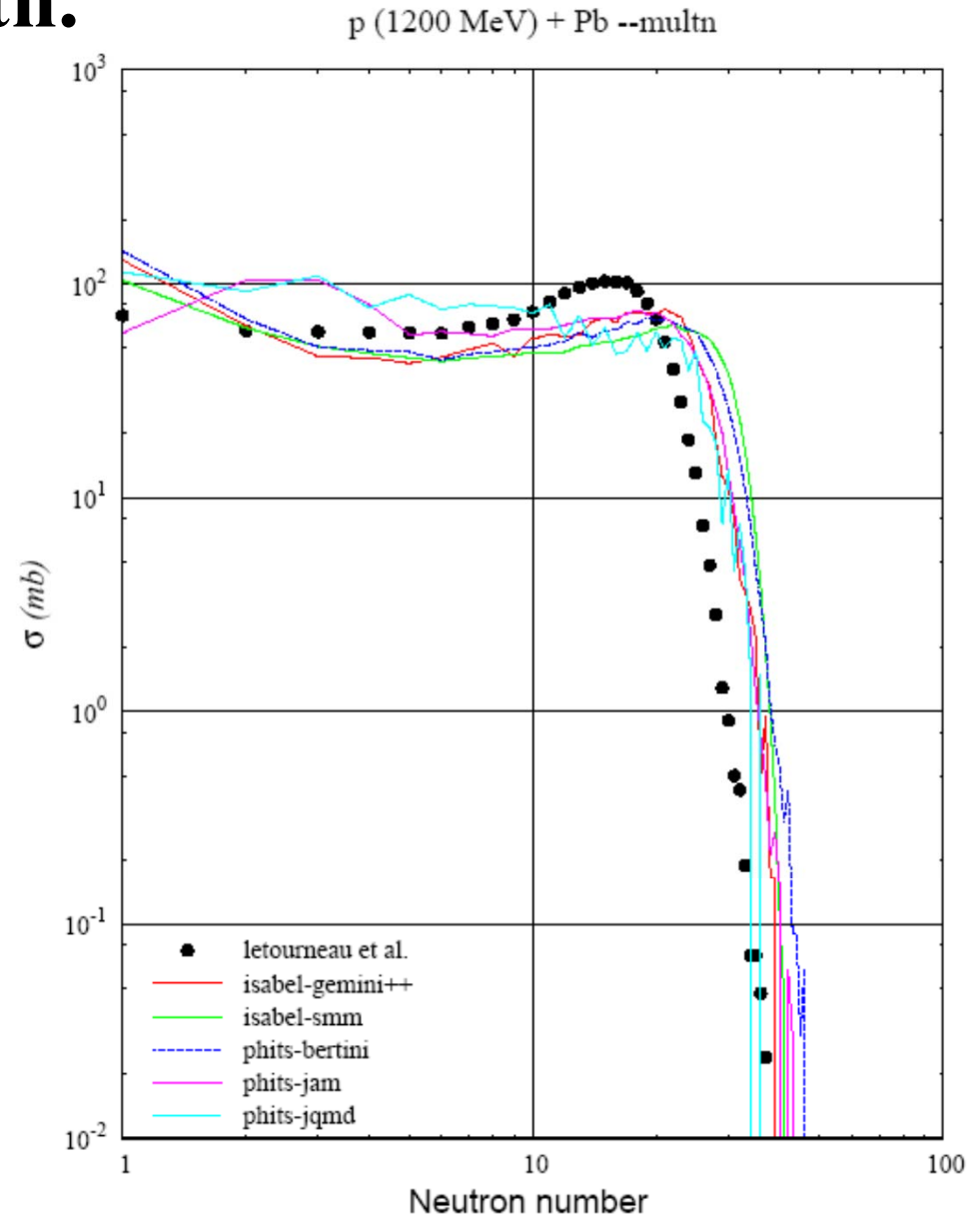


Pion minus production

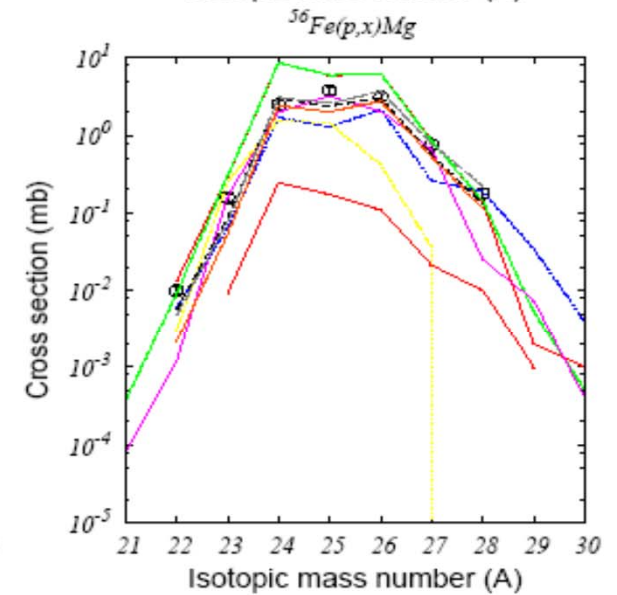
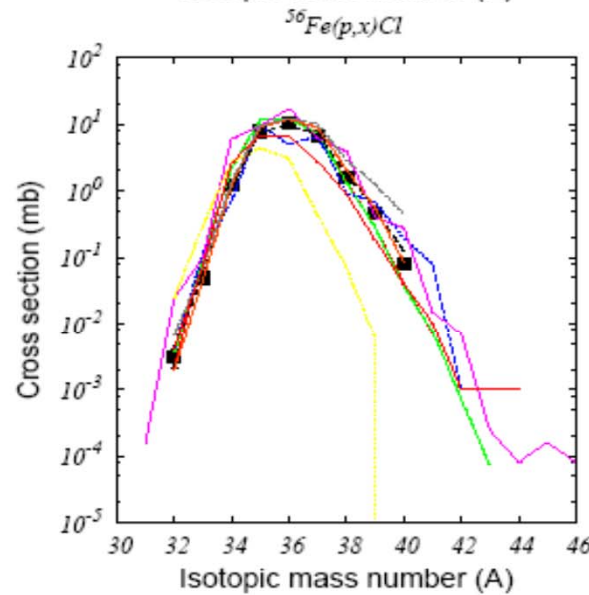
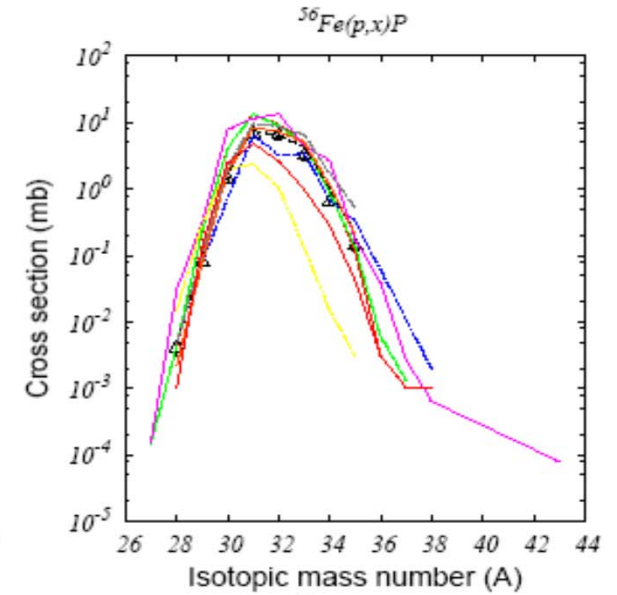
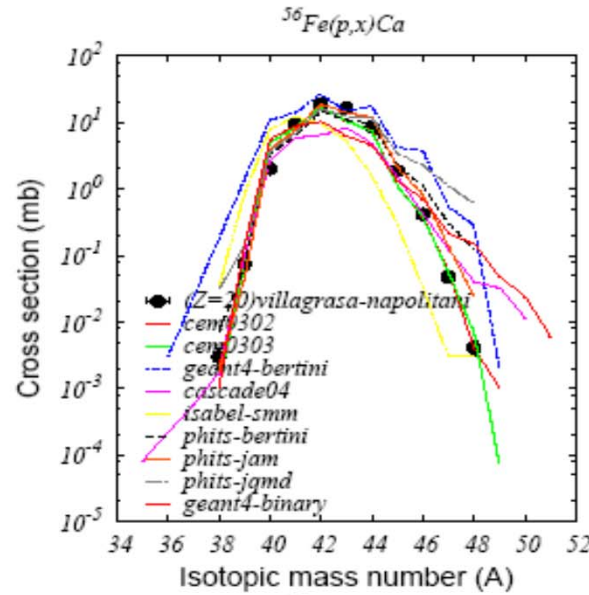


Neutron multiplicity distn.

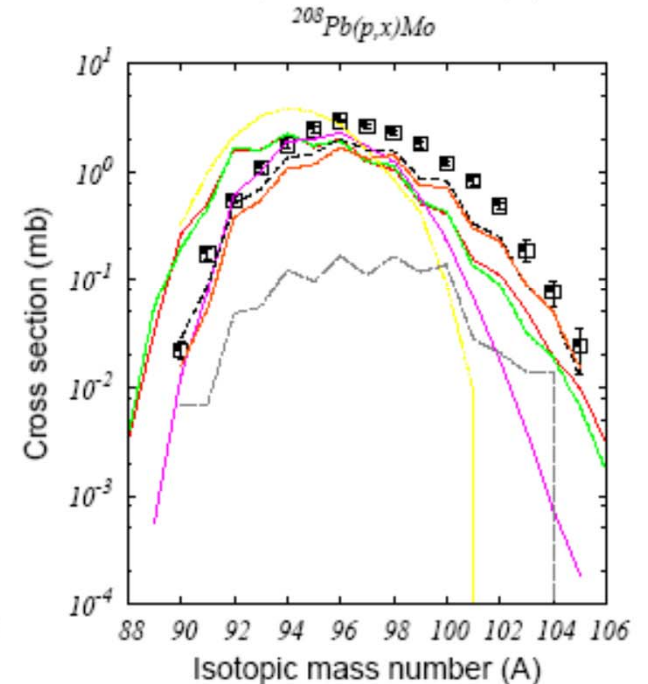
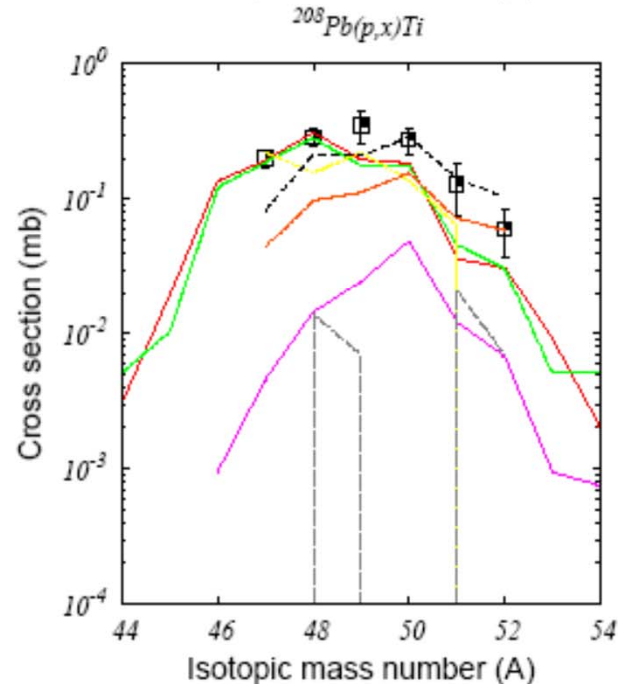
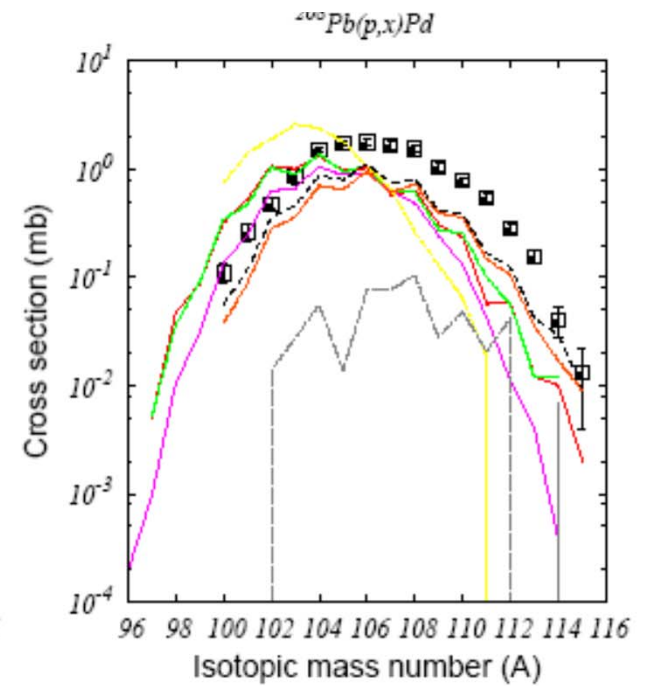
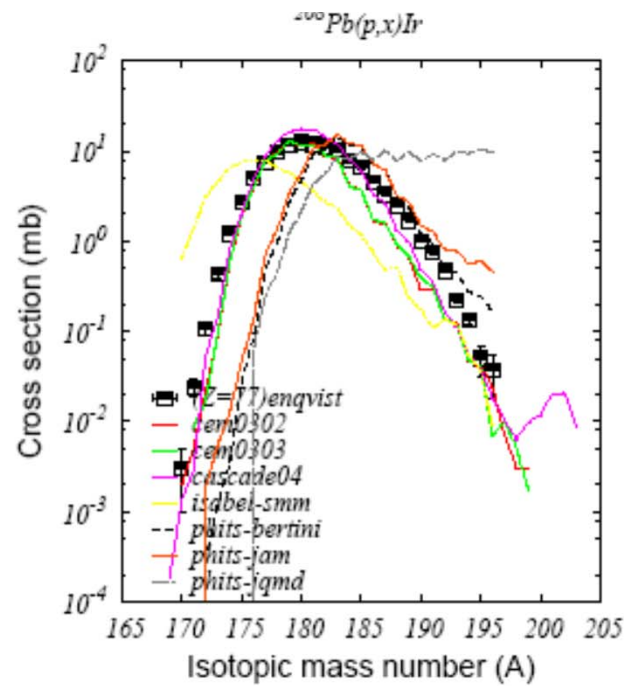
Data received from only
PHITS-jam,
PHITS-bertini,
PHITS-jqmd,
Isabel-smm,
Isabel-gemini models



Isotopic distn. for Fe target



Isotopic distn. for Pb target



6. Excitation function

Excitation function

Independent cross section (nuclear reaction only)

$$A(t) = N_T \sigma \Phi (1 - \exp(-\lambda t)), \quad 0 \leq t \leq t_{\text{irr}}$$

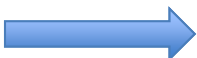
Cumulative cross section (nuclear reaction + decay of precursor(s))

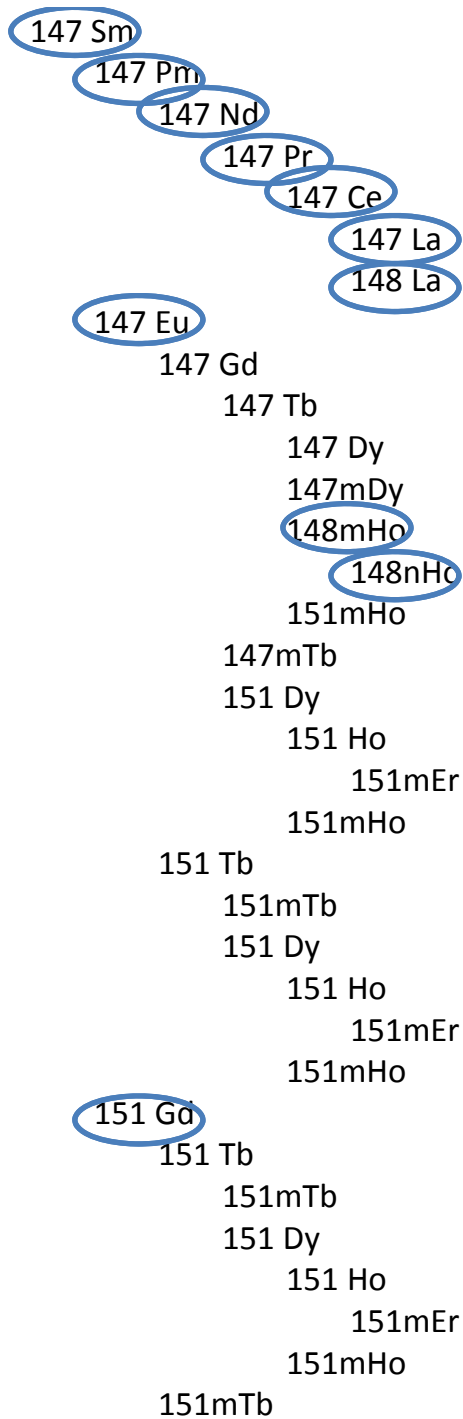
$$A_D(t) = N_T \Phi \left(\begin{aligned} &\left(\sigma_D + \sigma_M \frac{\lambda_M}{\lambda_M - \lambda_D} \right) (1 - \exp(-\lambda_D t_{\text{irr}})) \exp(-\lambda_D t) \\ &+ \sigma_M \frac{\lambda_D}{\lambda_M - \lambda_D} (1 - \exp(-\lambda_M t_{\text{irr}})) \exp(-\lambda_M t) \end{aligned} \right)$$

$\sigma = ???$

IF $\lambda_M \gg \lambda_D$ \longrightarrow $\sigma_C = \left(\sigma_D + \sigma_M \frac{\lambda_M}{\lambda_M - \lambda_D} \right)$

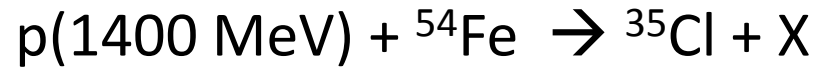
Excitation function

- Half-lives / Branching ratios: decay data library of DCHAIN-SP (EAF-3.1, FENDL/D-1, ENSDF, ...)
- $\lambda_M \gg \lambda_D$ (???)  T_M/T_D ratio can be changed

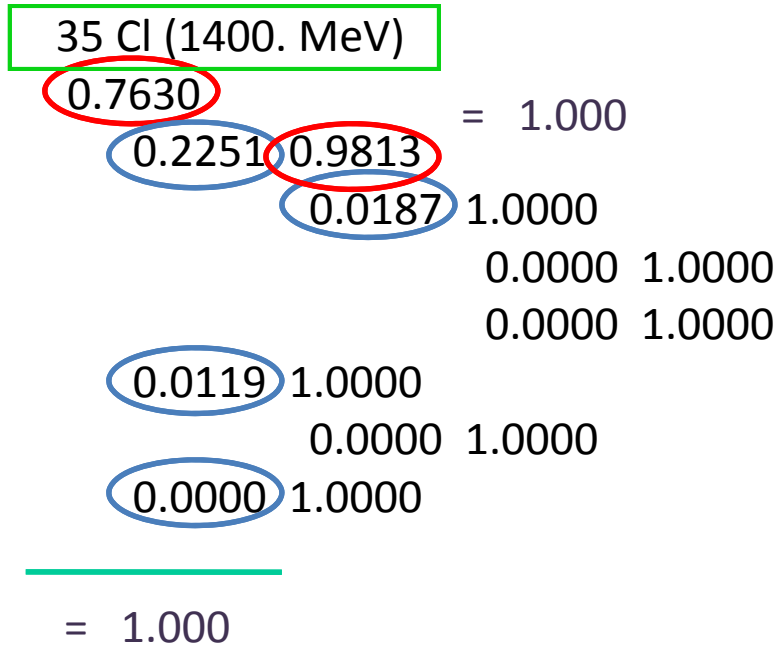


Example

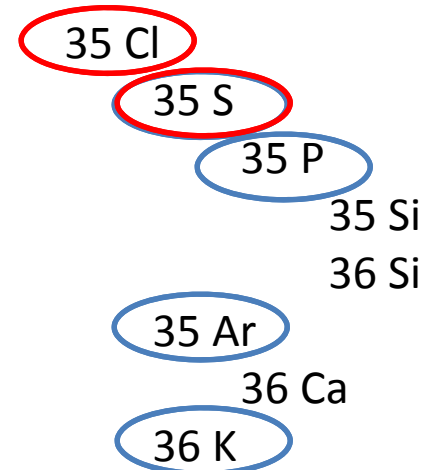
^{147}Sm Precursors ($T_M/T_D = 0.1$)



Contribution to σ_c



Progenitor Chain



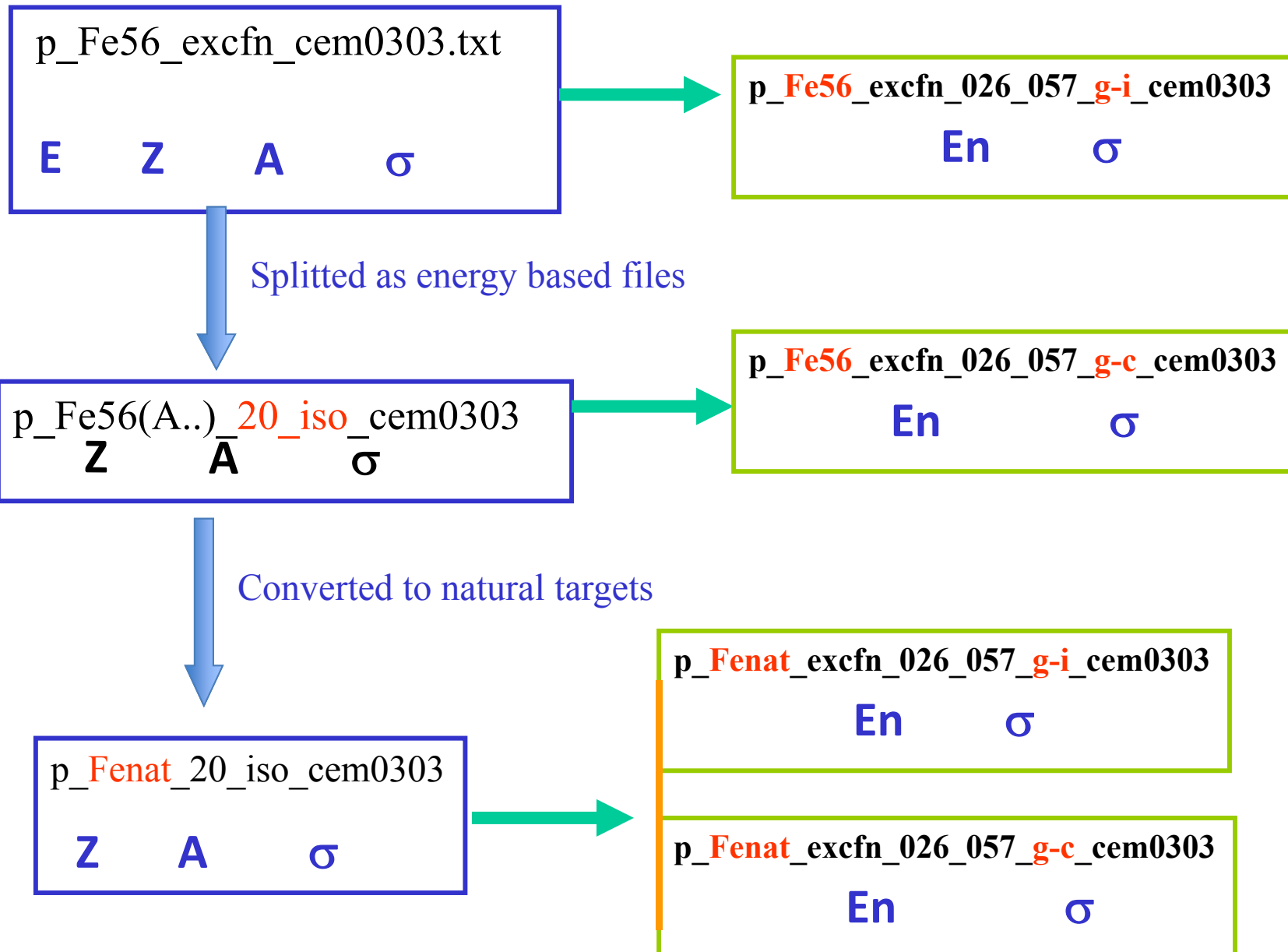
- nuclear reaction
- decay of precursor(s)

Status of the excitation function data

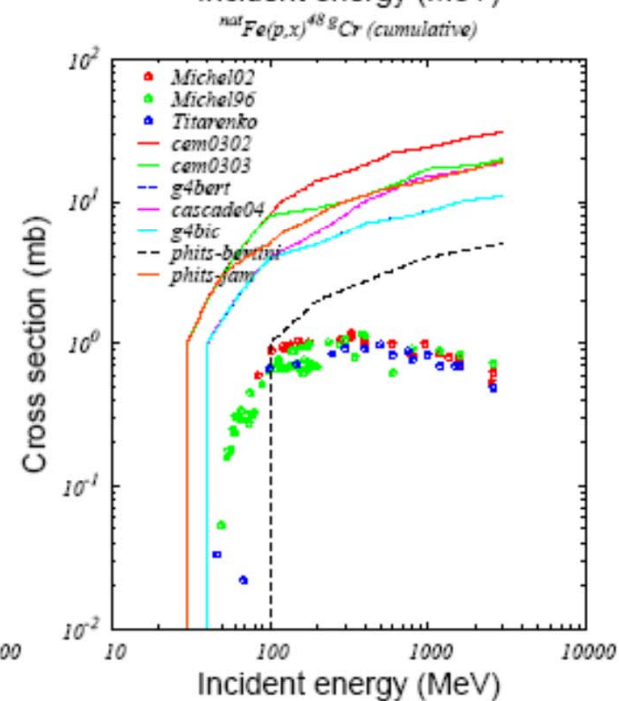
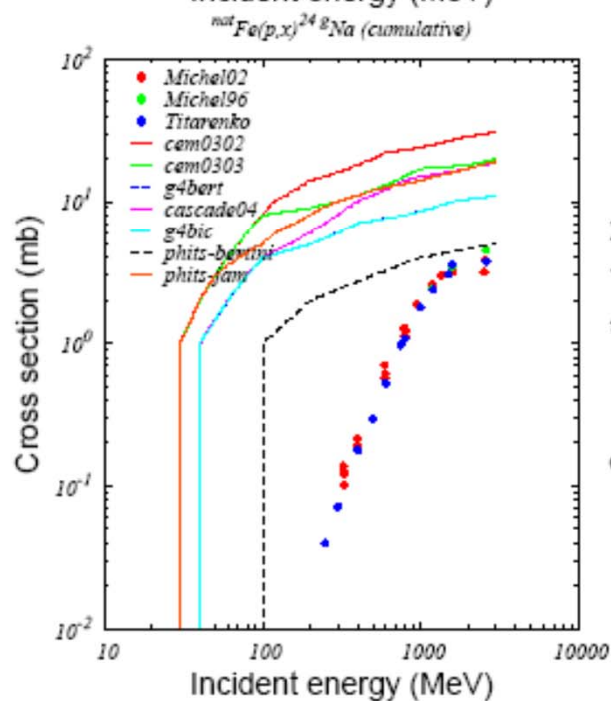
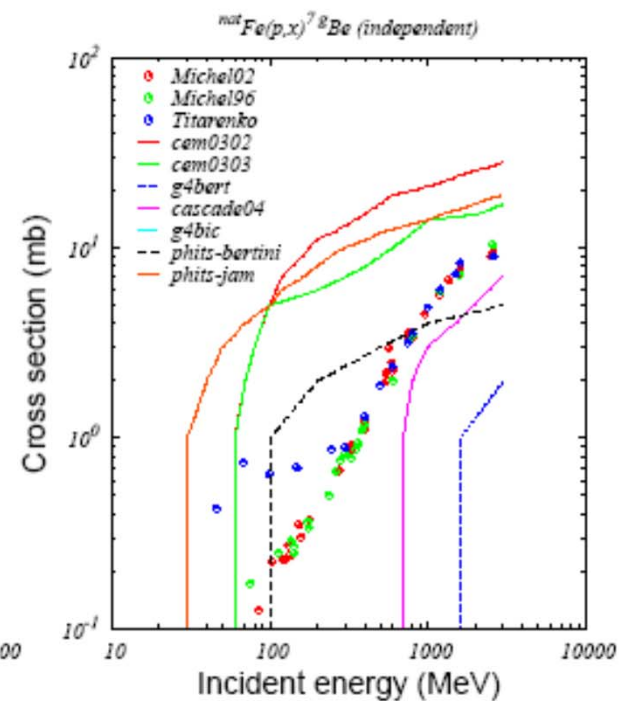
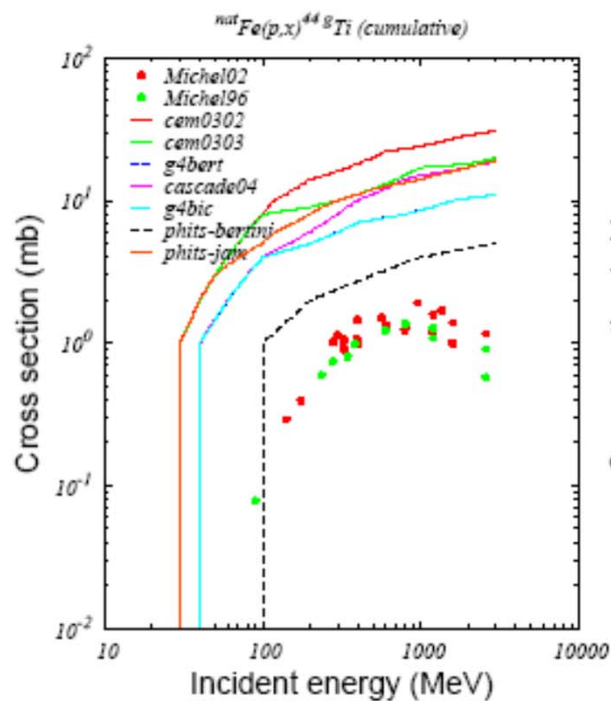
Codes	Given data as
CEM0302	p_Fe56_20_iso_cem03_02 Z A σ dσ
CEM0303	p_Fe56_excfn_cem0303 E Z A σ dσ
Cascade04	p_Fe56_20_iso_cascade04 Z A σ dσ
PHITS-jam*	p_Fe_50_iso_phits(JAM)
PHITS-bertini*	p_Pb_50_iso_phits(Bertini) Z A σ
Geant4-binary	p_Fenat_20_excfn_g4bic
Geant4-bertini	p_Pbnat_20_excfn_g4bert Z A σ dσ

* PHITS provided independent & cumulative data separately. We just arranged them as excitation function data.

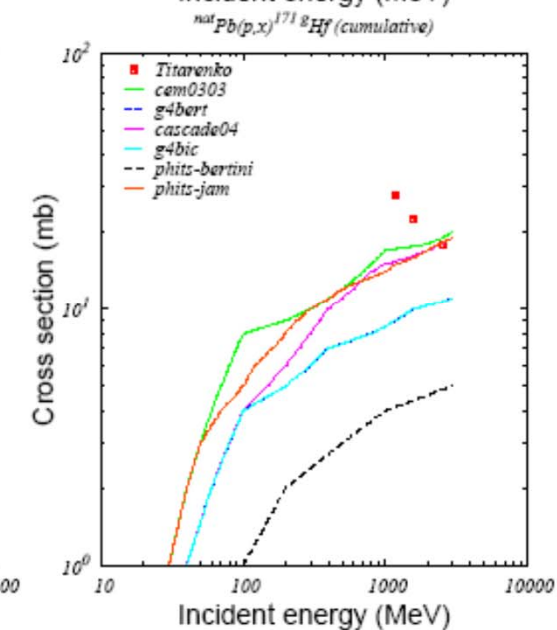
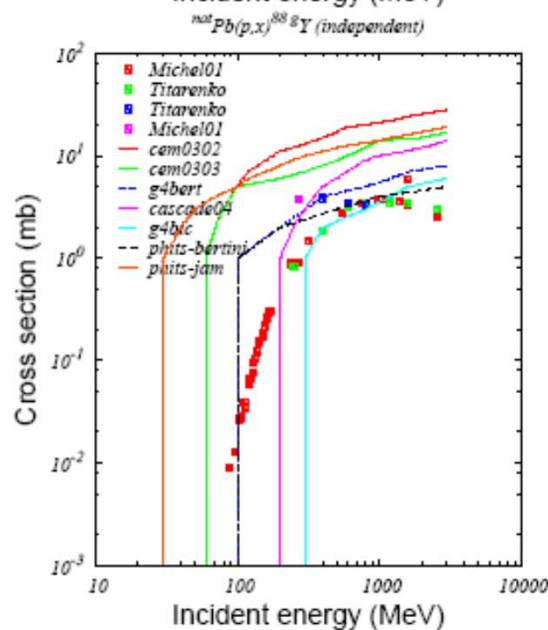
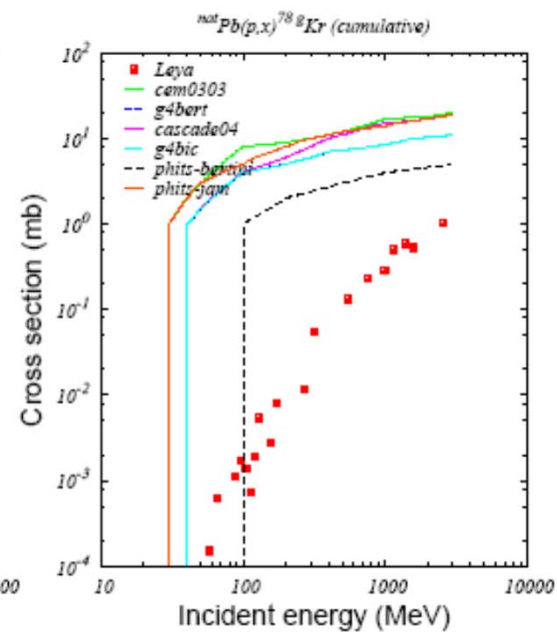
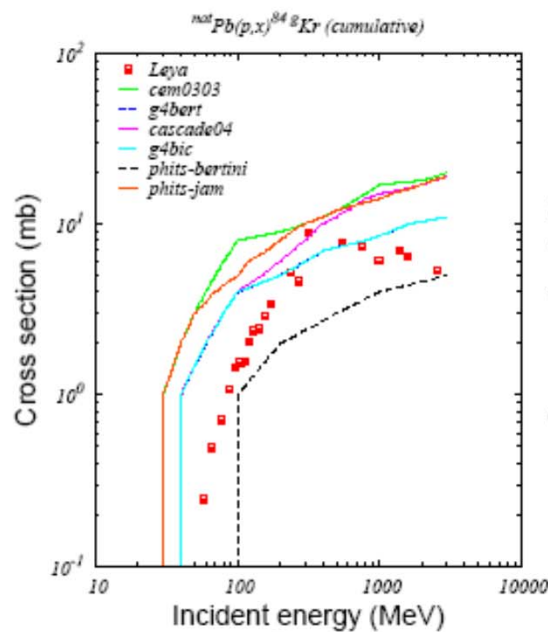
Excitation function Data processing



Excitation function from natFe target



Excitation function from natPb target



General/preliminary outcomes

1. **Neutron emission** → Most of the models prediction **apparently** similar.
2. **Proton emission** → Overall good reproduction of experimental data by some models, except few reaction systems.
3. **Composite particles** (d, t, he-3, he-4..) → Most of the models have deviation to experimental data around a factor of 2 or higher.
4. **Pion production** → Reproduce overall similar to exp. data by all models.

General/preliminary outcomes

- 5. **Neutron multiplicity distn.** → Well predicted by the given models (PHITS-all, Isabel-all)
- 5. **Isotopic distribution** → Shows overall good prediction by most of the models
- 5. **Excitation function** → Most of the models prediction shows clear discrepancy

Plan to do work on.....

Figure of Merit

→ Statistical analysis: Calculation of deviation factor ?

→ Chi-square fitting & parameter ?

Time frame for Benchmarking of Spallation Models

1. Final deadline for submission of calculations
→ **July 31, 2009**
2. Meeting of the Evaluation Panel Committee
→ **1st week, October'09; at IAEA**
3. Final report on Benchmarking on Spallation Models
→ **by November 2009**
4. Workshop: Physics on Intercomparison
→ **February, 2010; at ICTP**
5. Presentation of Intercomparison Results
→ **Nuclear Data Conf., 2010; Korea**