# Tools for Benchmarking of Spallation Models & -First results

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## 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. | Ingre-dients |
|---|---|---|---|---|---|---|---|---|
| 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<br>Affiliation : Liege University, CEA Saclay, GSI Darmstadt |
| **INCL4+GEMINI** | Participants: J Cugnon, A Boudard, R Charity<br>Affiliation: Liege University, CEA Saclay, University of S Louis |
| **INCL4+SMM** | Participants: J Cugnon, A Boudard, A Botvina<br>Affiliation: Liege University, CEA Saclay, Russian Academy of Science |
| **ISABEL+ABLA** | Participants: Y Yariv, A Kelic<br>Affiliation: Soreq NRC, GSI-Darmstadt |
| **FLUKA*** | Participants: A Ferrari<br>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

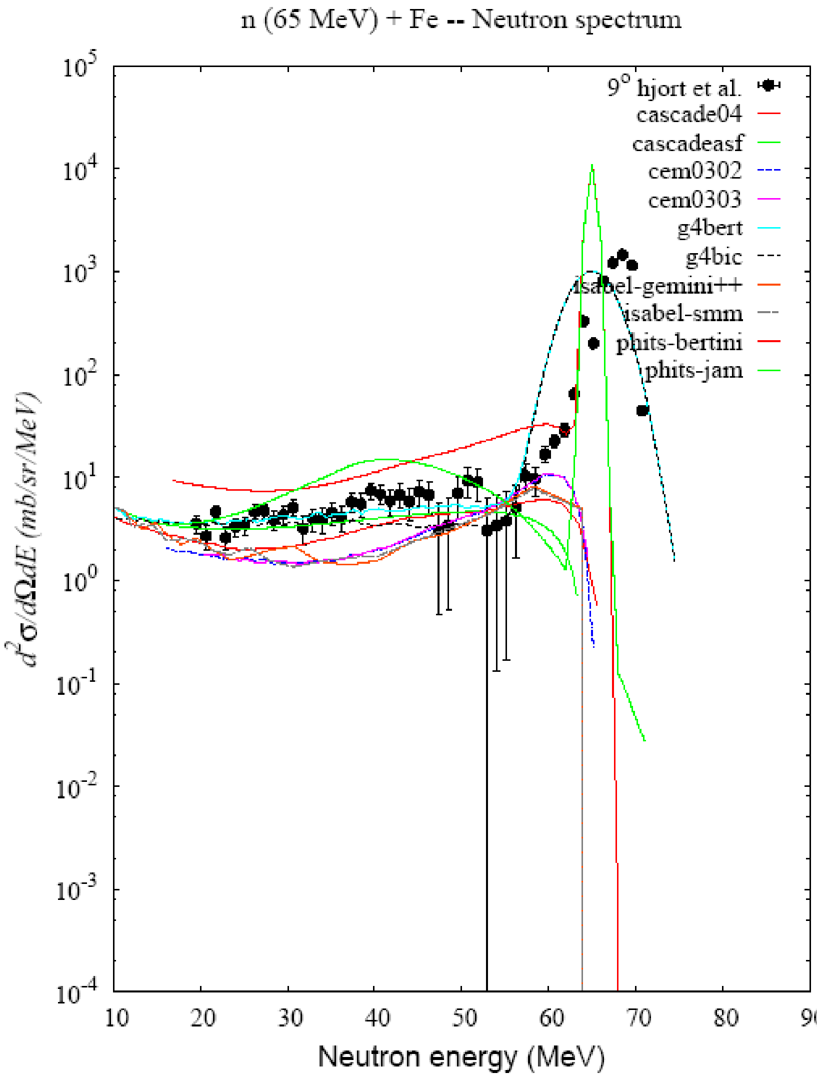
**Experimental data**
**versus**
**Any combination of model calculations**

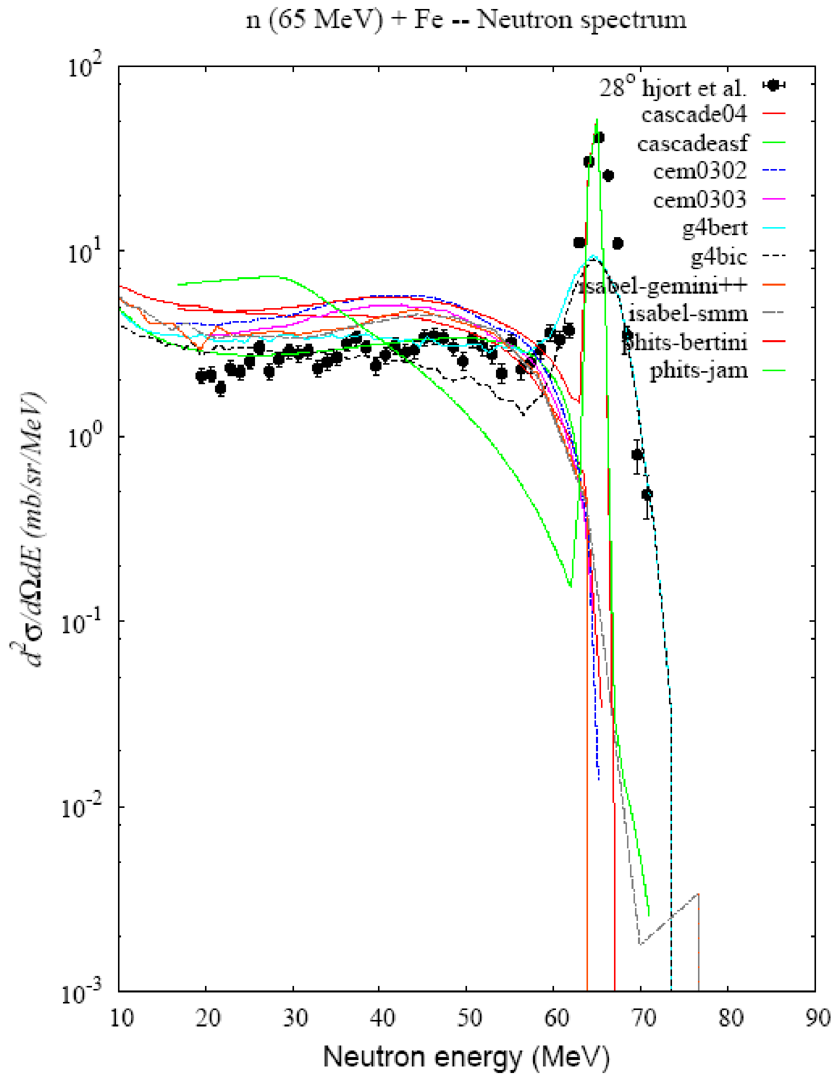
Examples → Exp. data vs. all angle / model #1
→ Exp. data vs. all angle / model #1, #2, #3,..
→ Exp. data vs. one angle / model #1
→ Exp. data vs. one angle / model #1, #2, #3,..

# 1. Neutron Spectrum

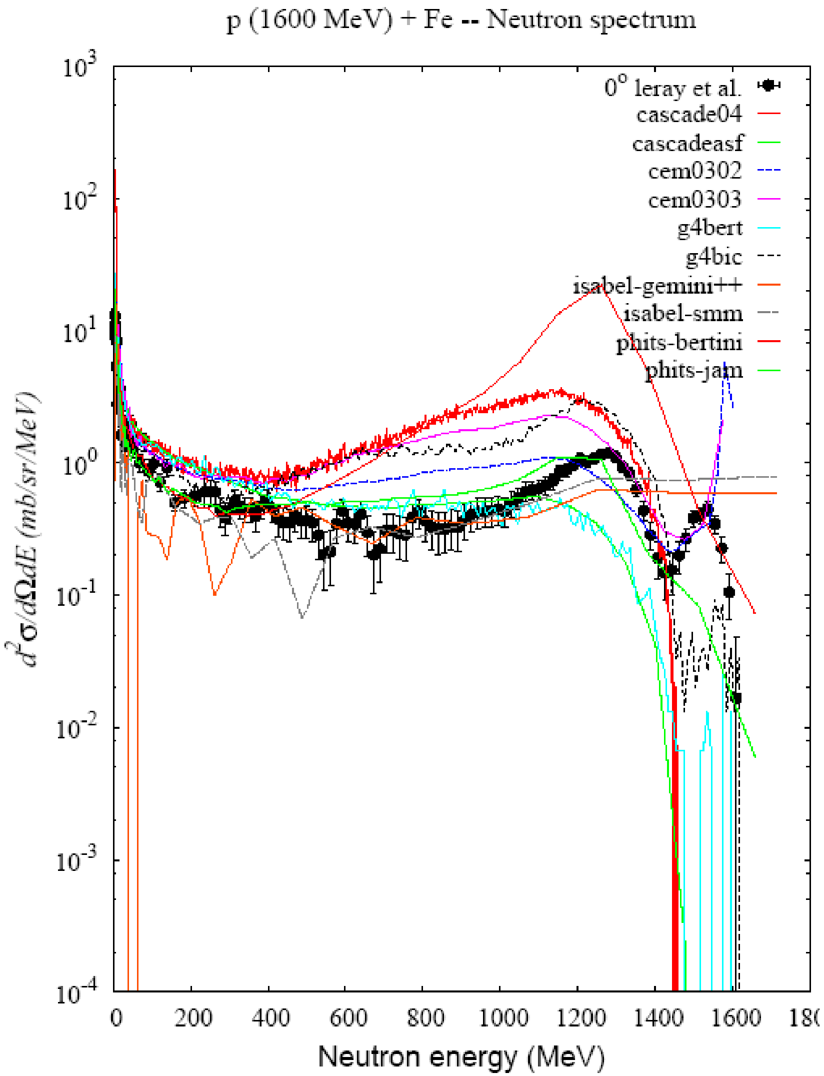
## Examples

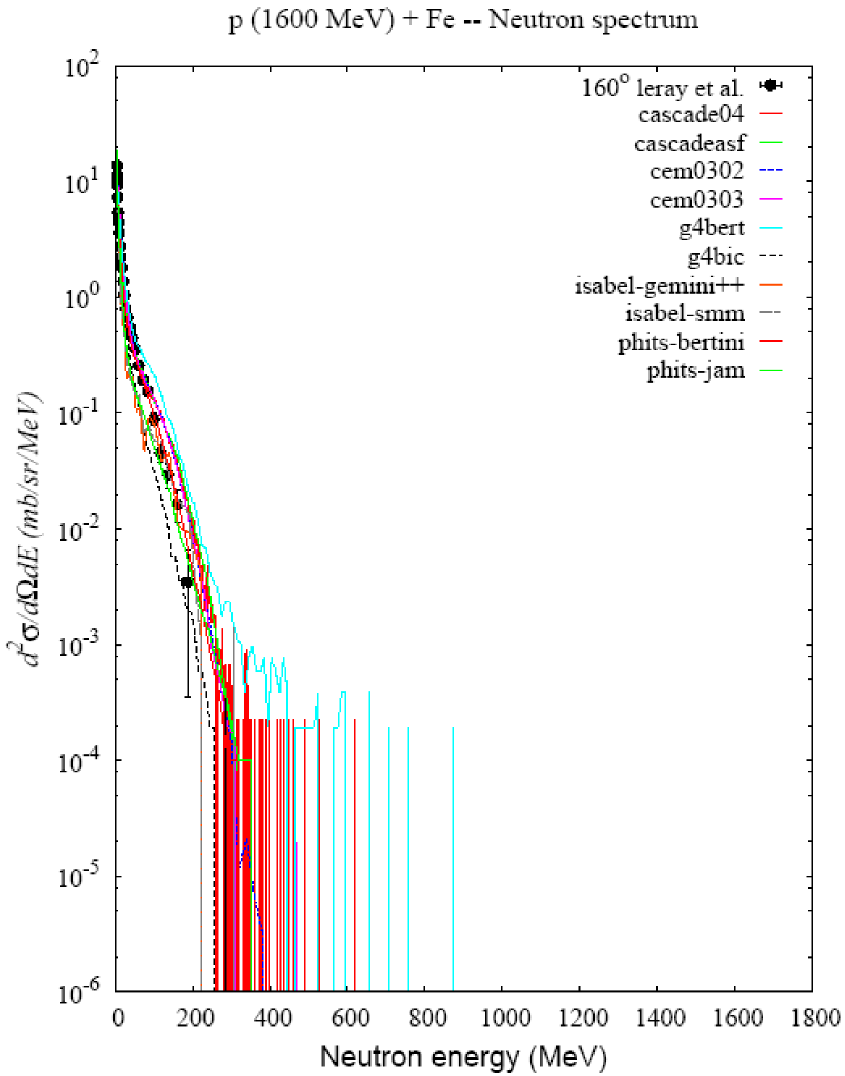
# Neutron spectrum with low energy projectile



# 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

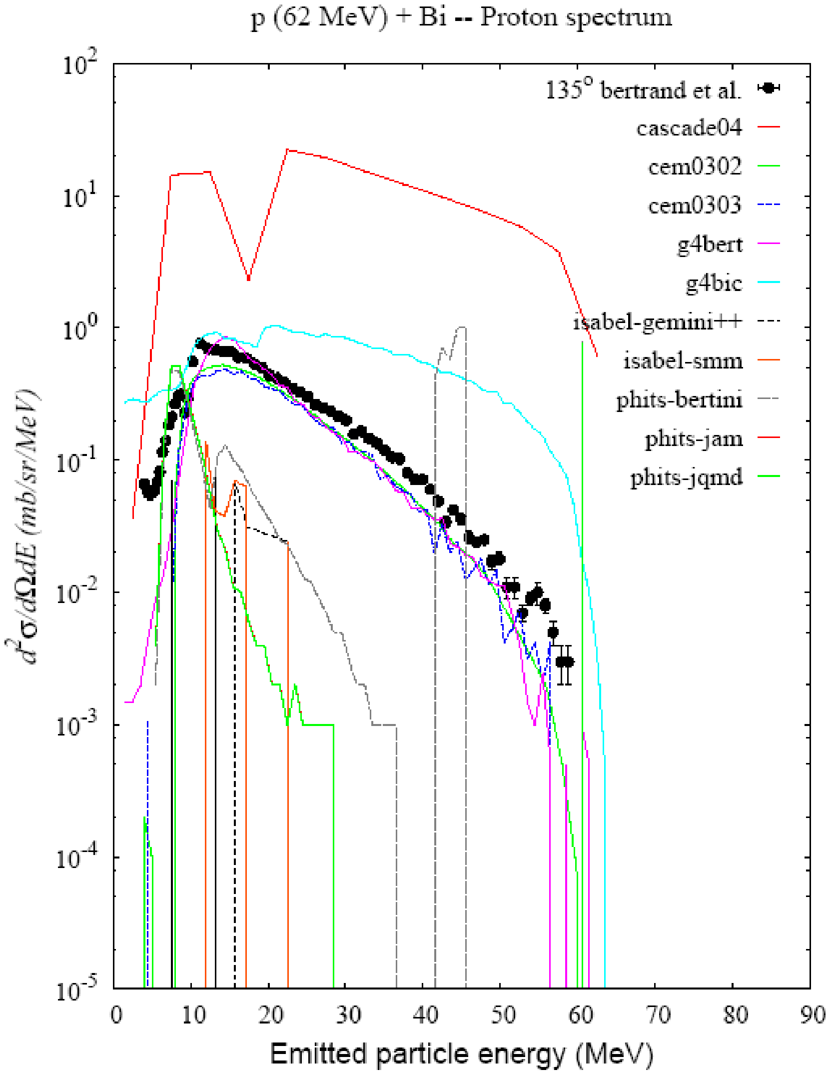
http://www-nds.iaea.org/spallations/

# 2. Light Charged Particle production

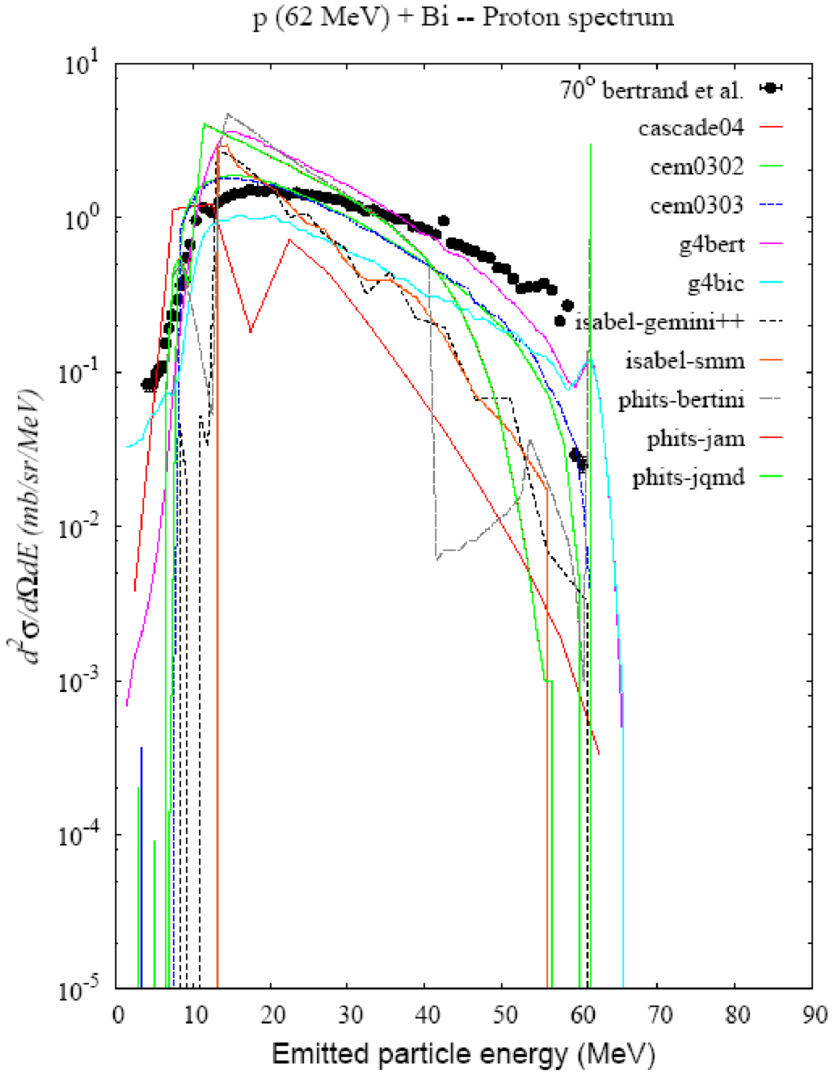
## Examples

# Proton Spectrum with low energy projectile

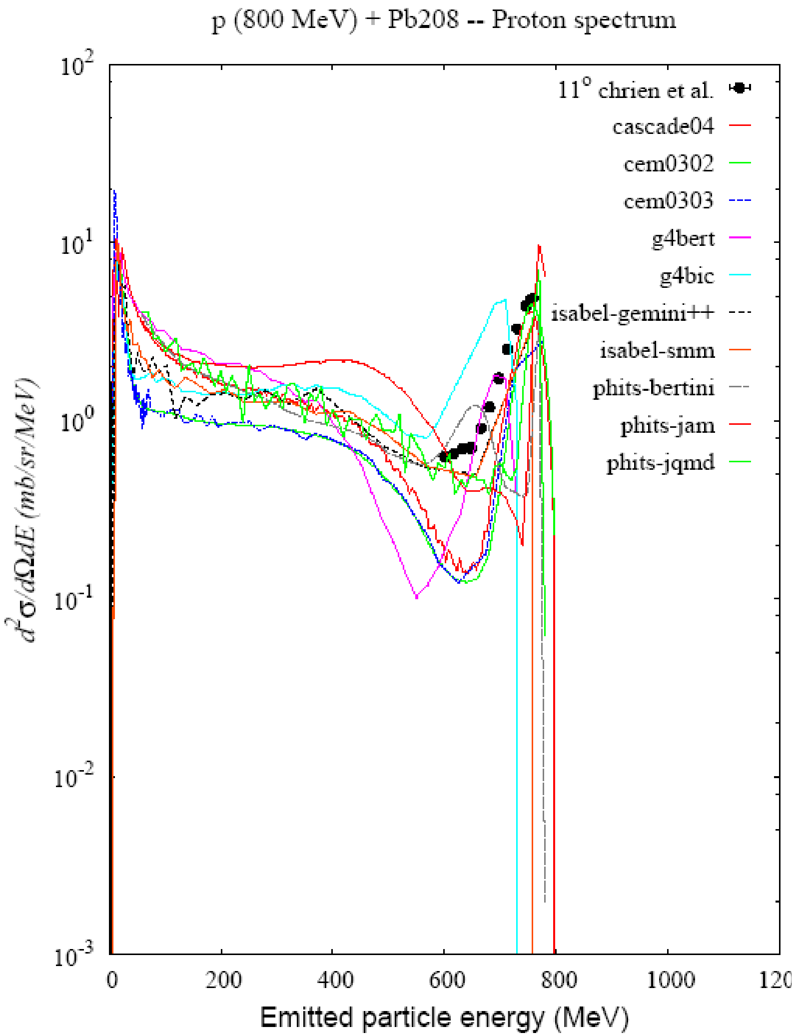
## Overestimated

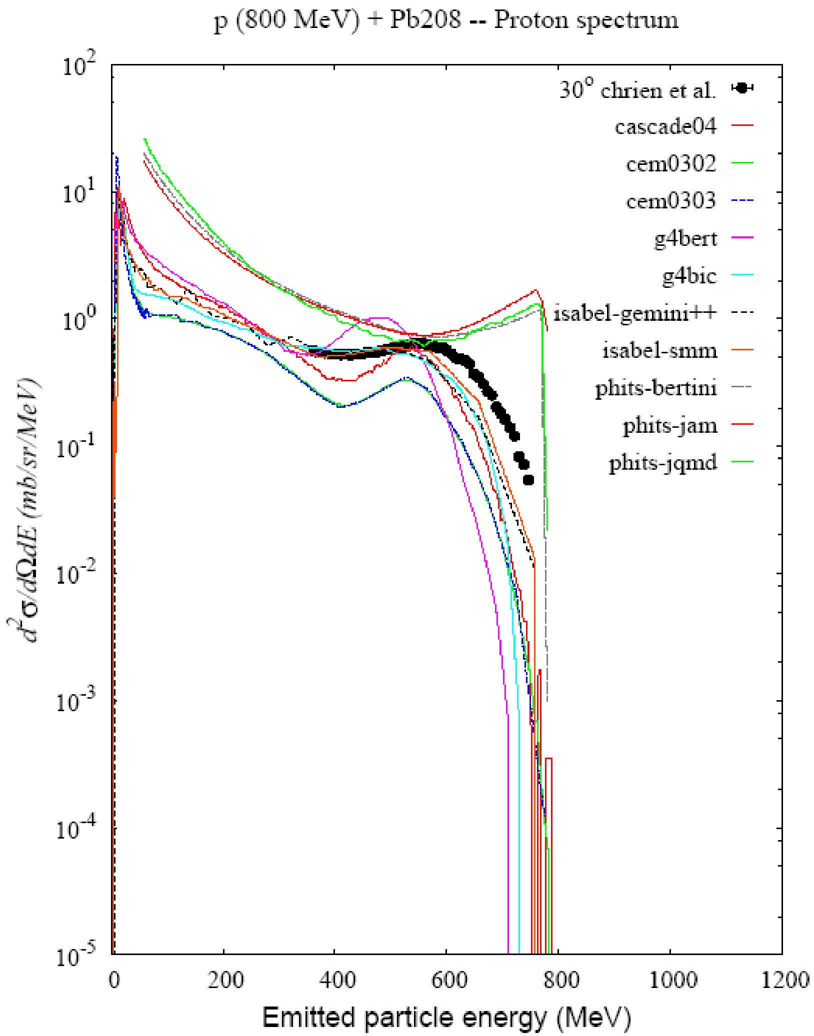



## Underestimated



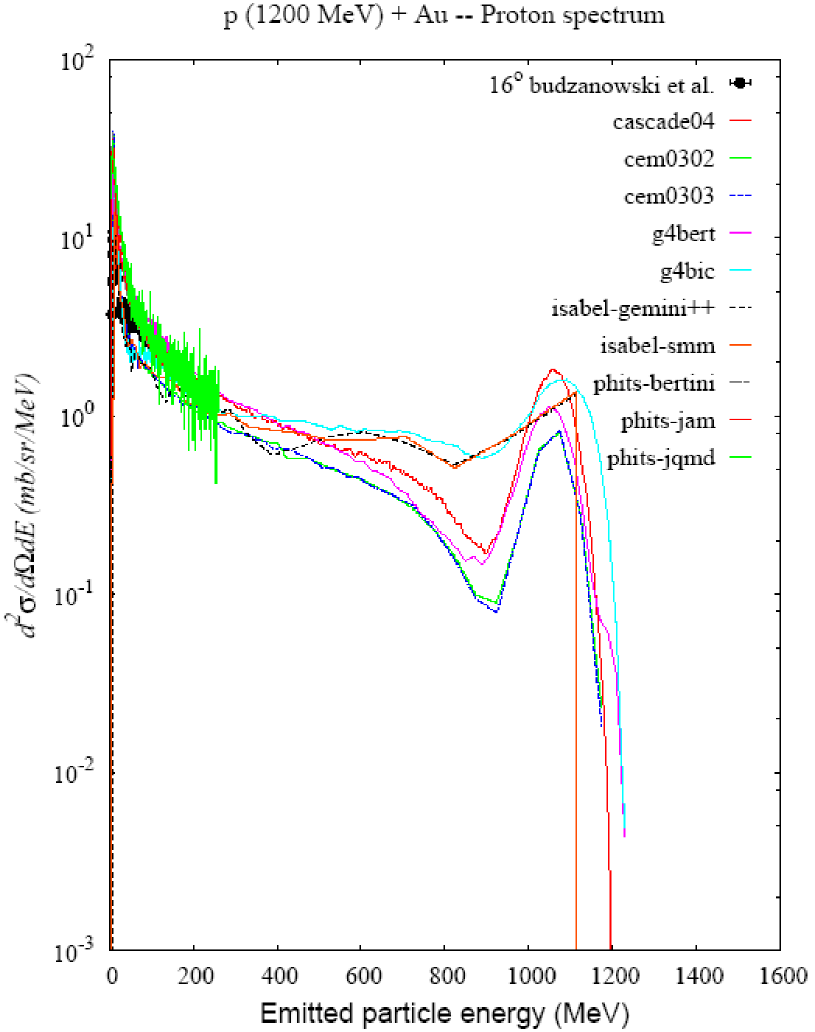
# Proton Spectrum with high energy projectile



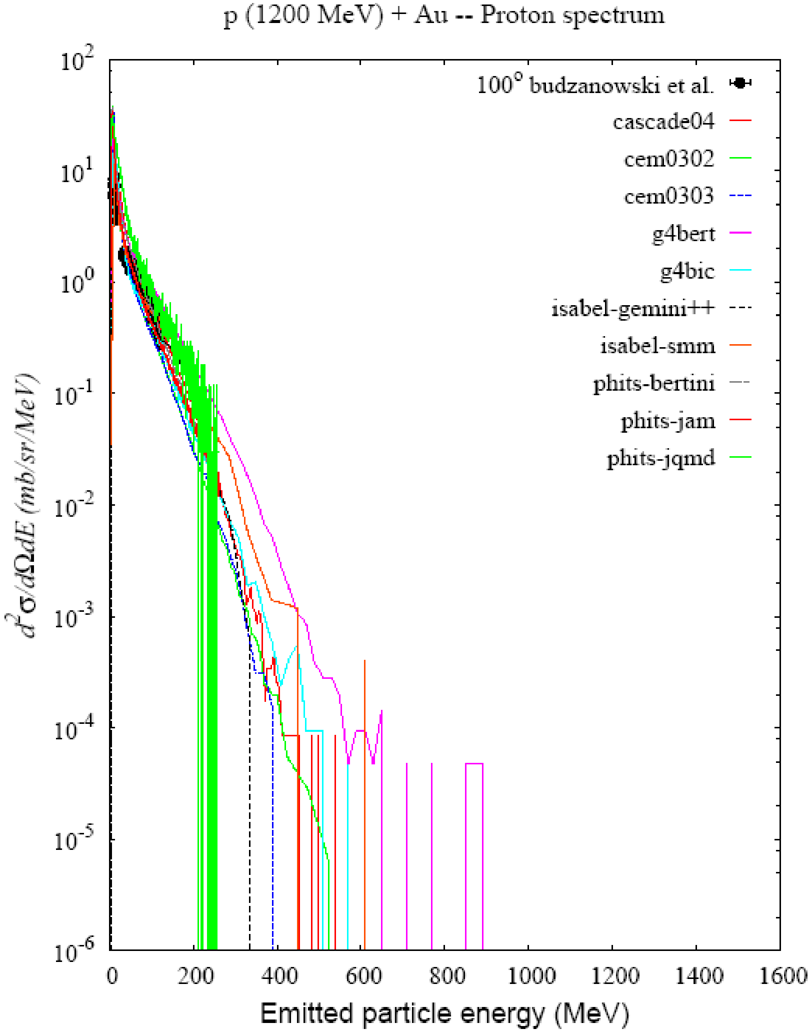



# Proton Spectrum with high energy projectile

## Forward angle

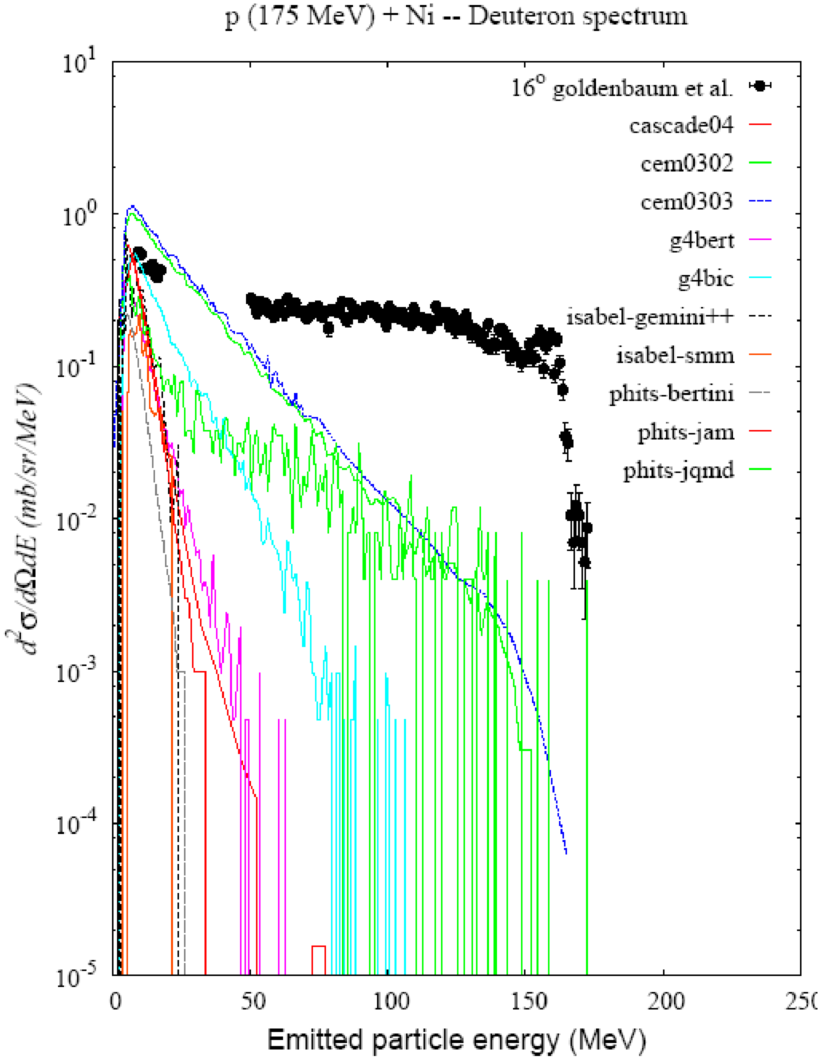



## Backward angle

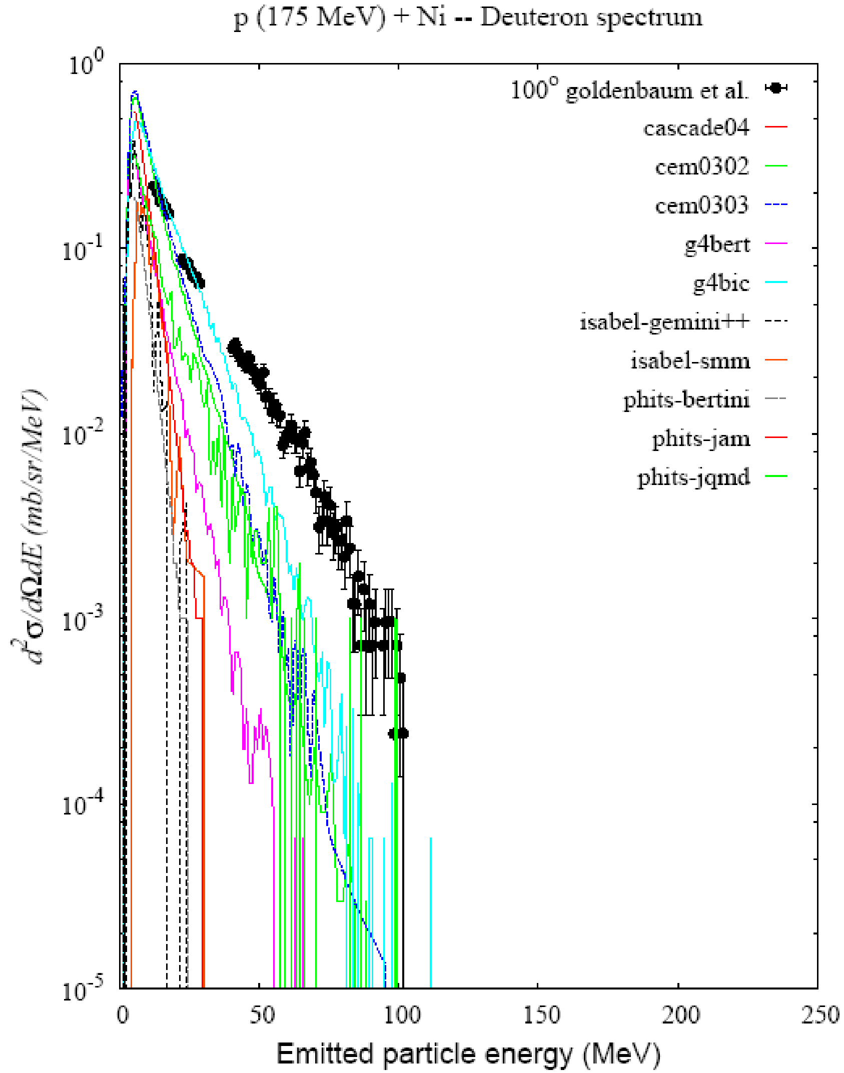


# Deuteron Spectrum with medium energy projectile

Forward angle

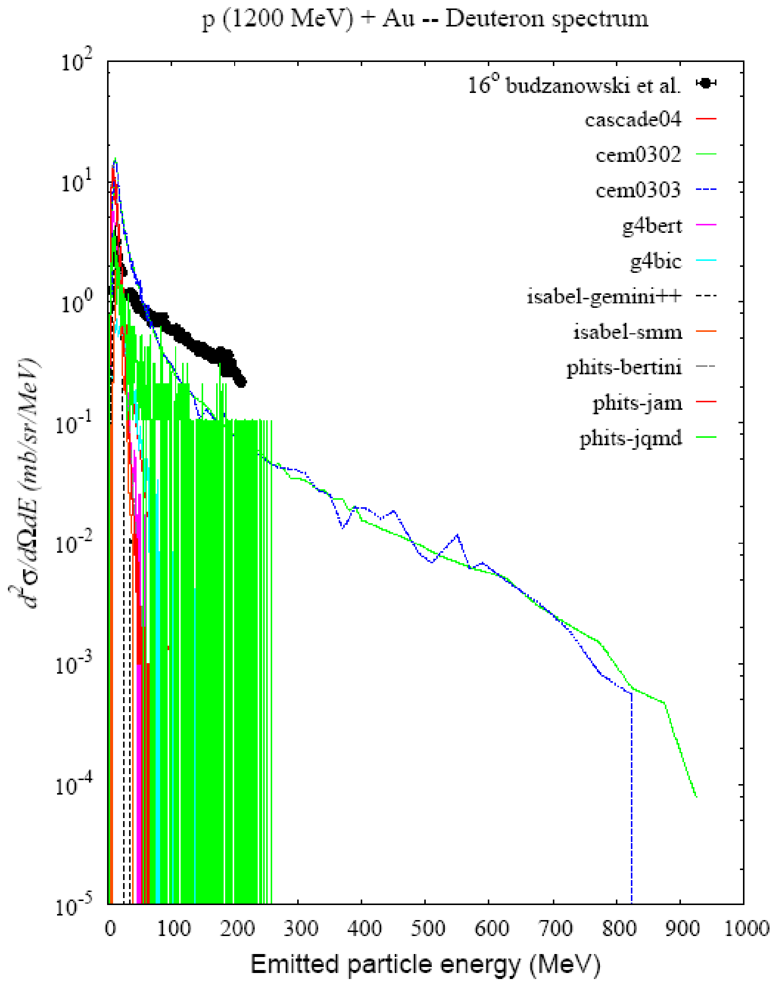



Backward angle

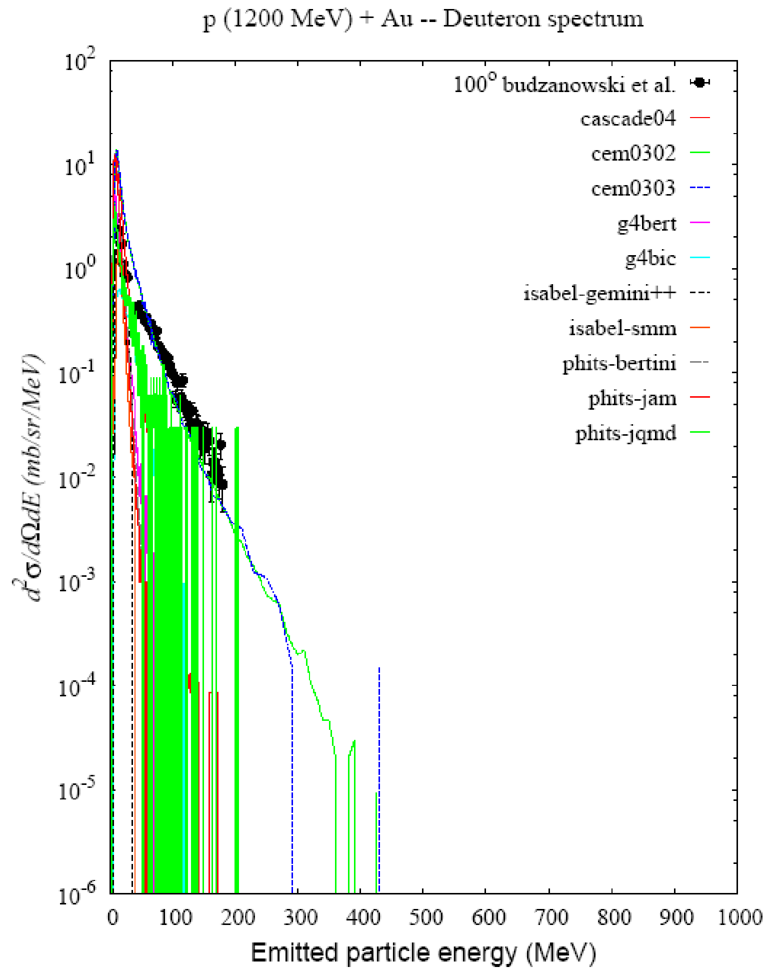


# Deuteron Spectrum with high energy projectile

## Forward angle

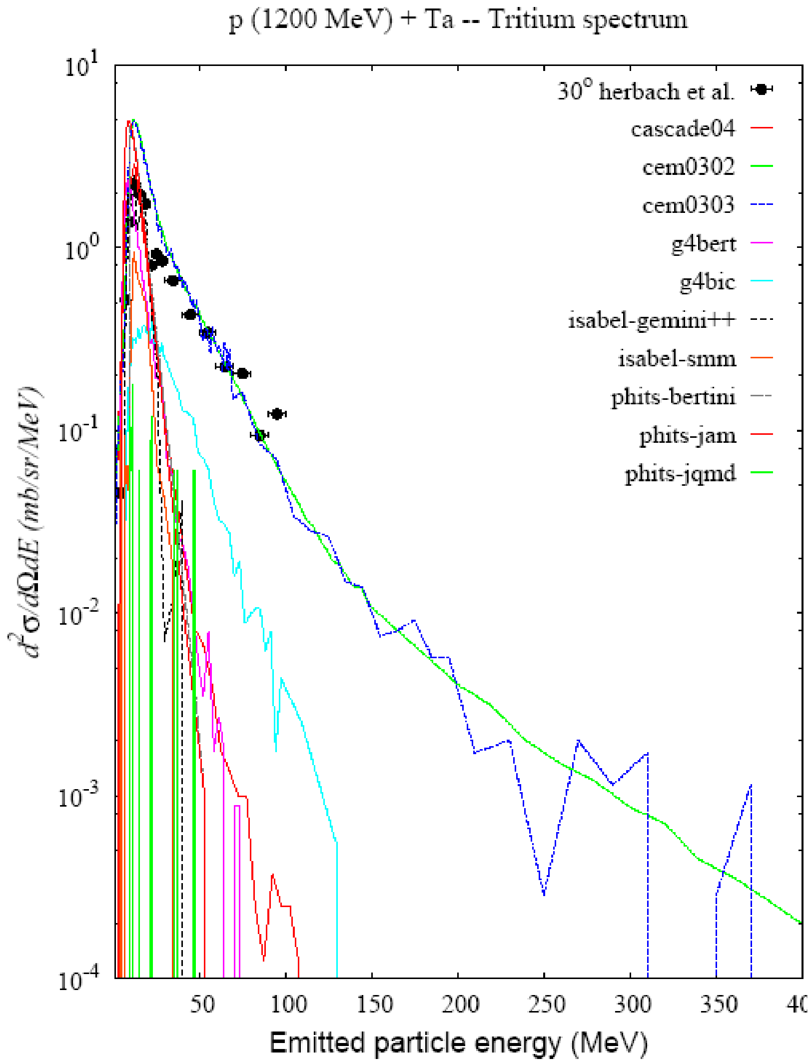



## Backward angle

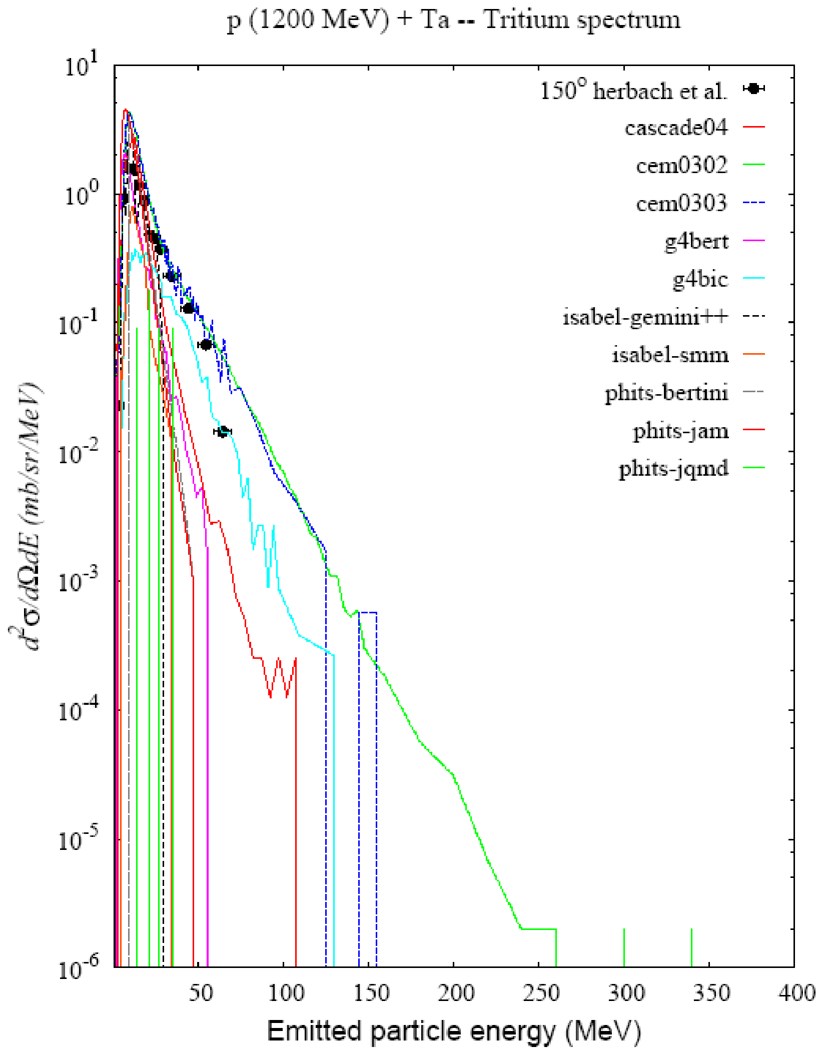


# Tritium Spectrum with high energy projectile

## Forward angle

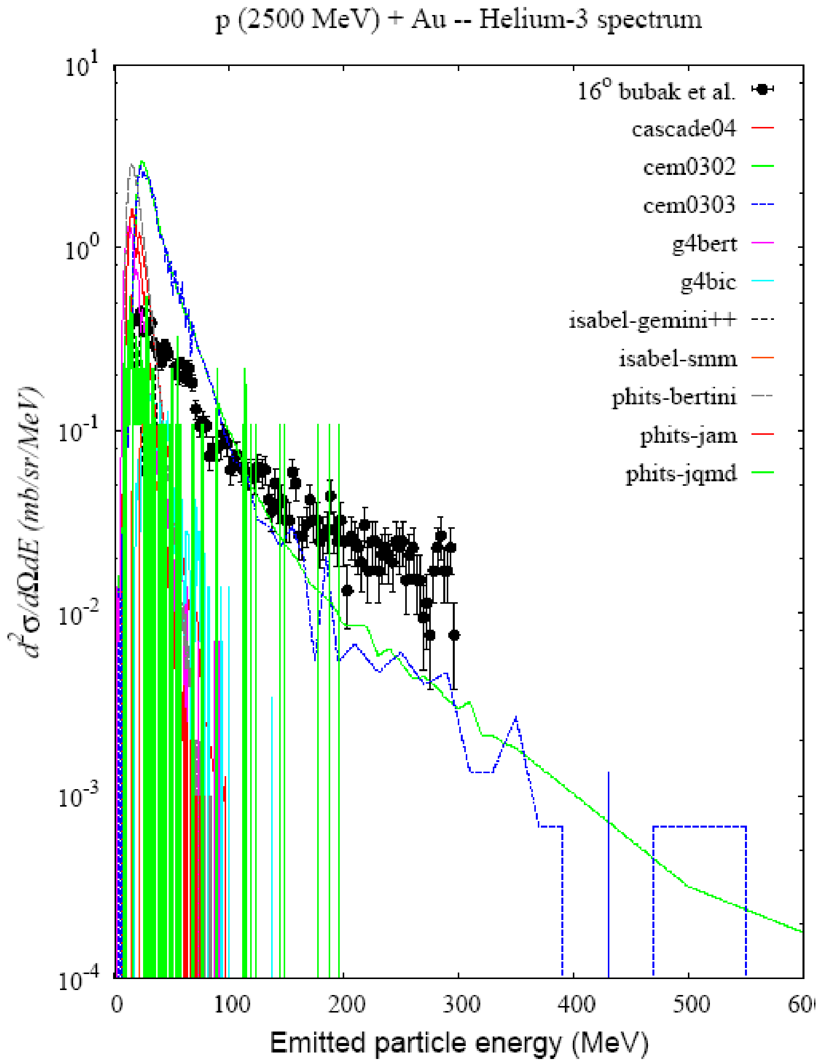



## Backward angle

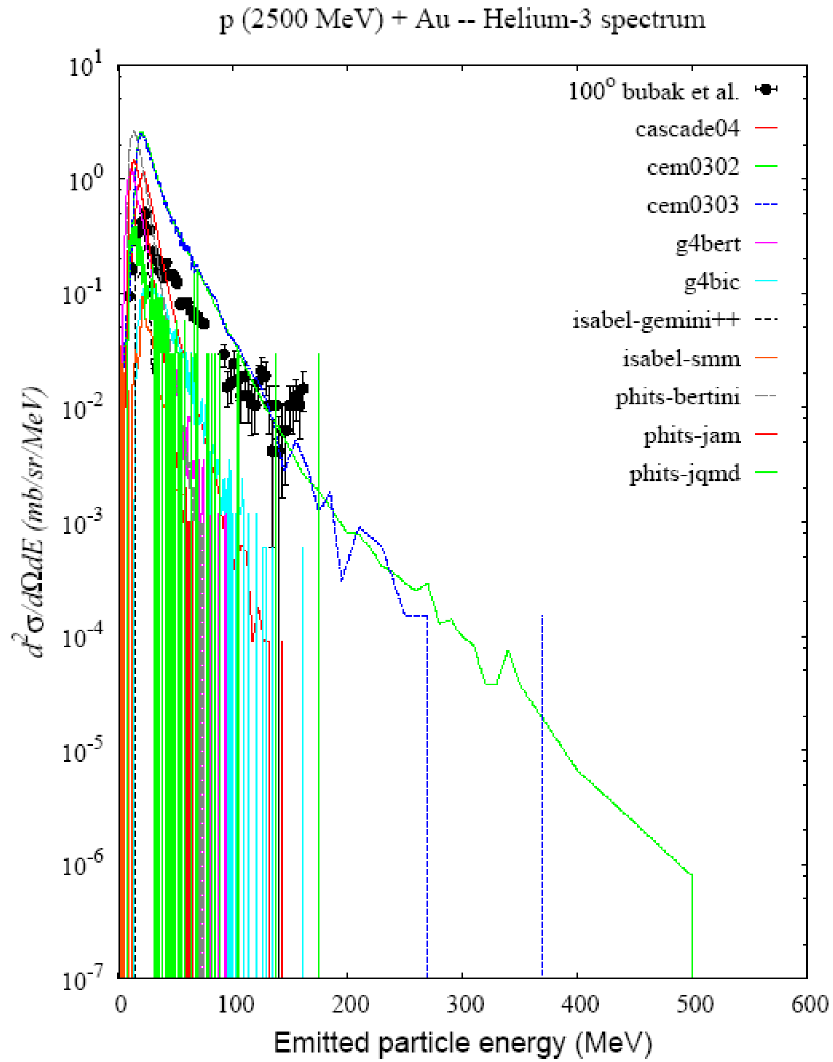


# Helium-3 Spectrum with high energy projectile

## Forward angle

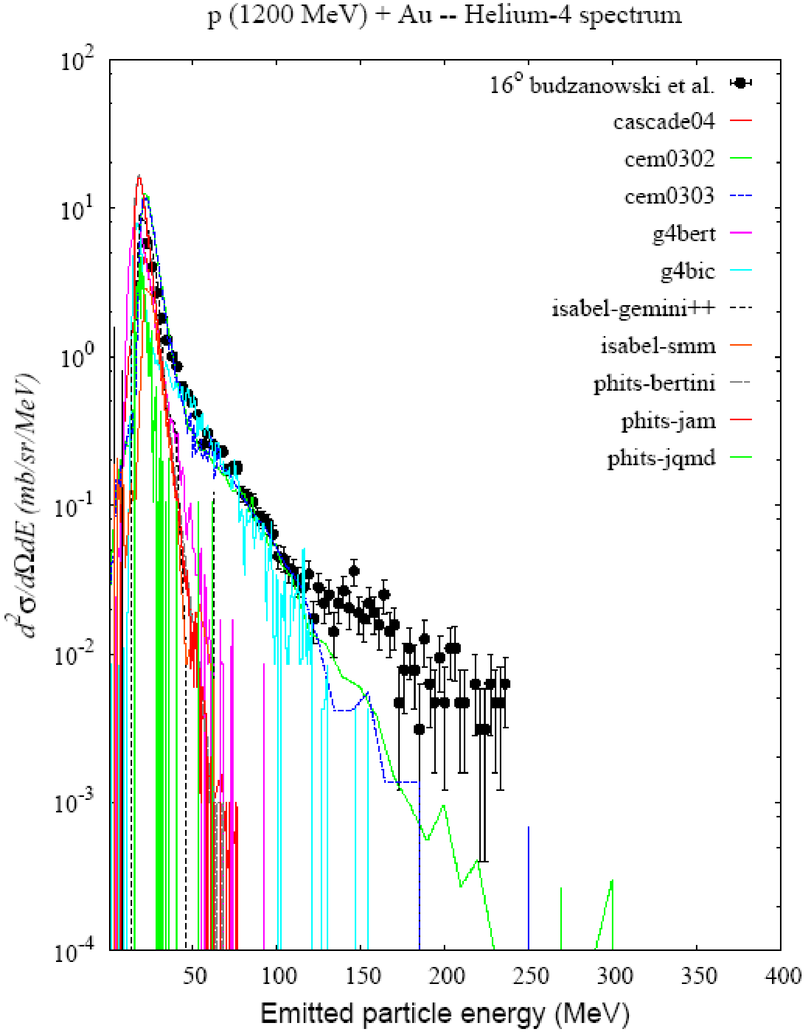



## Backward angle

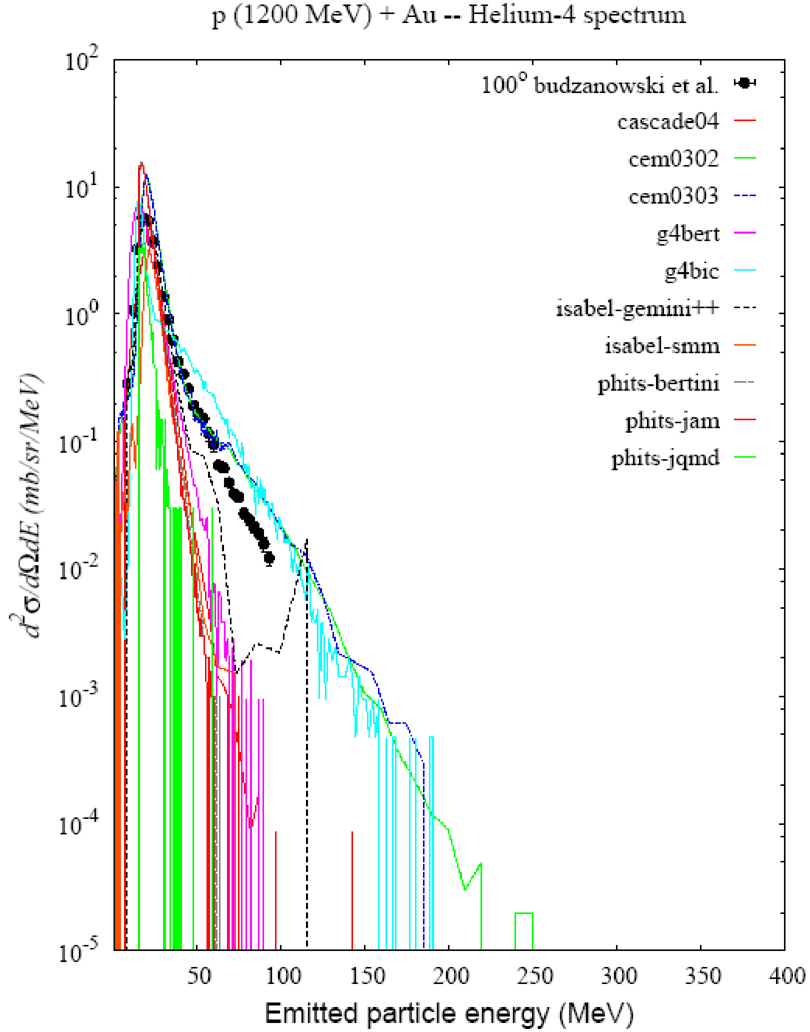


# Alpha Spectrum with high energy projectile

## Forward angle

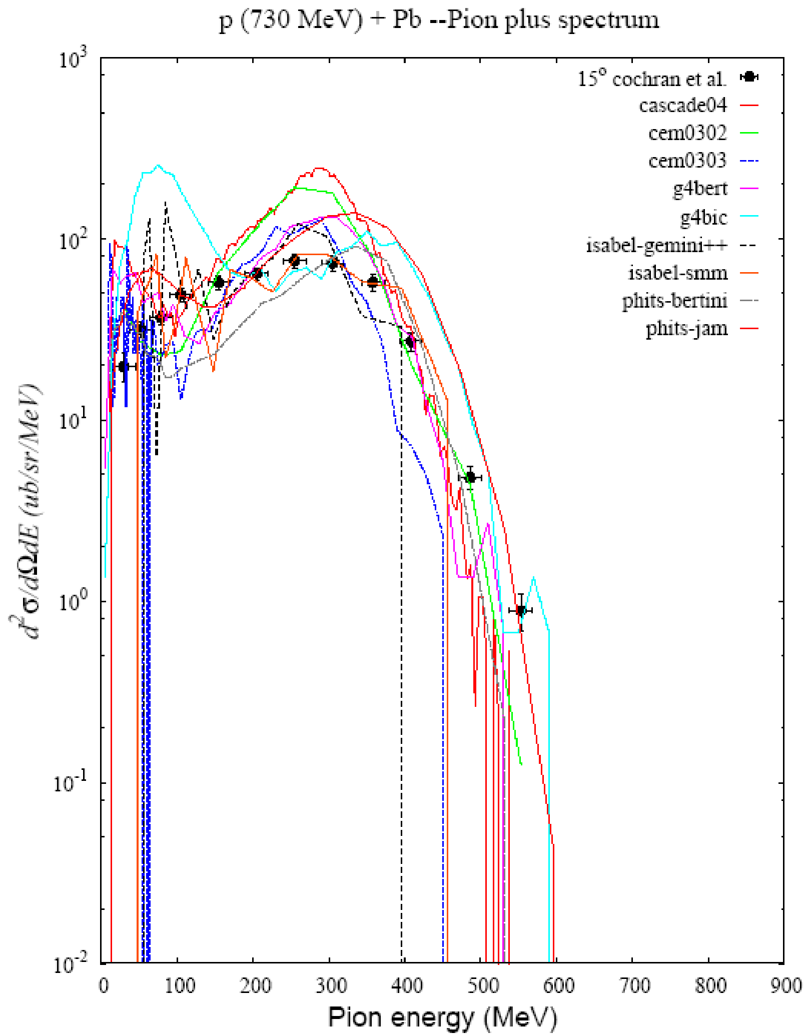



## Backward angle

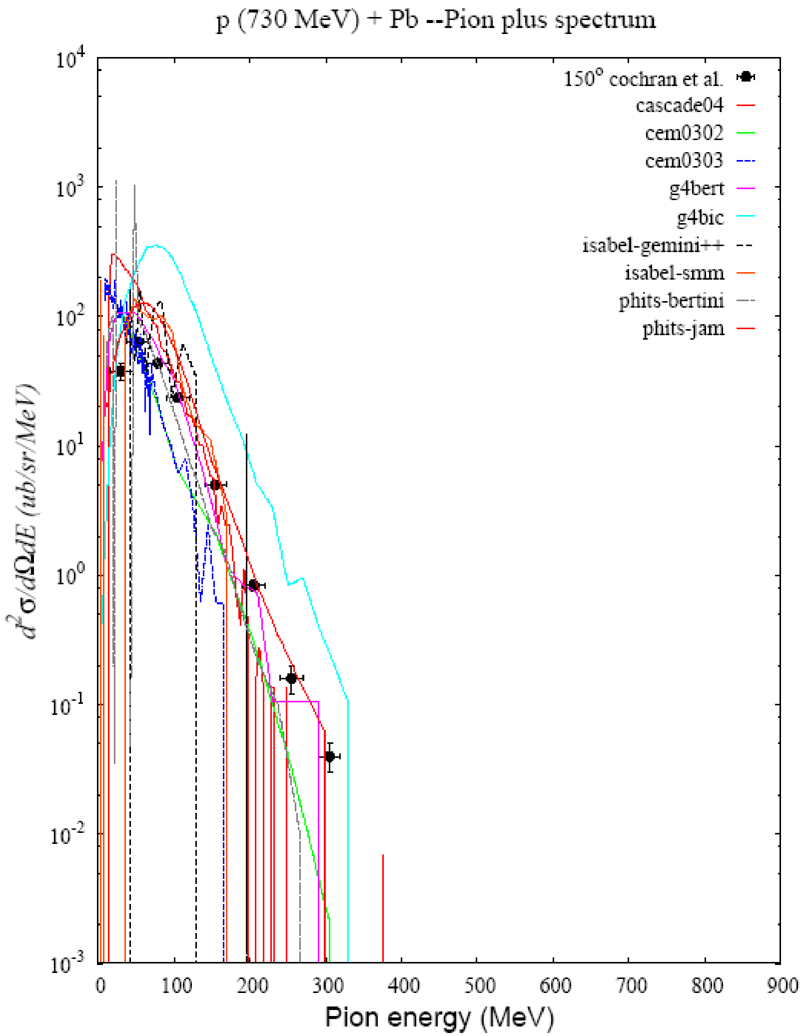


# Pion plus production

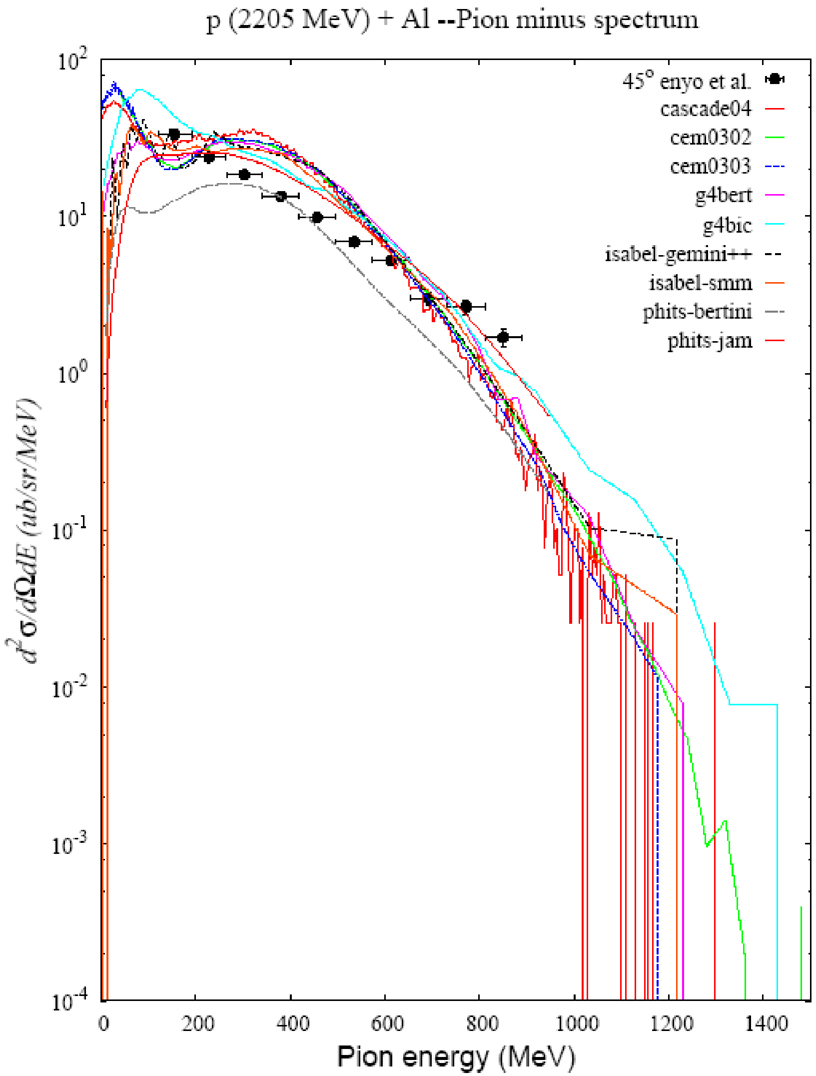
## Forward angle

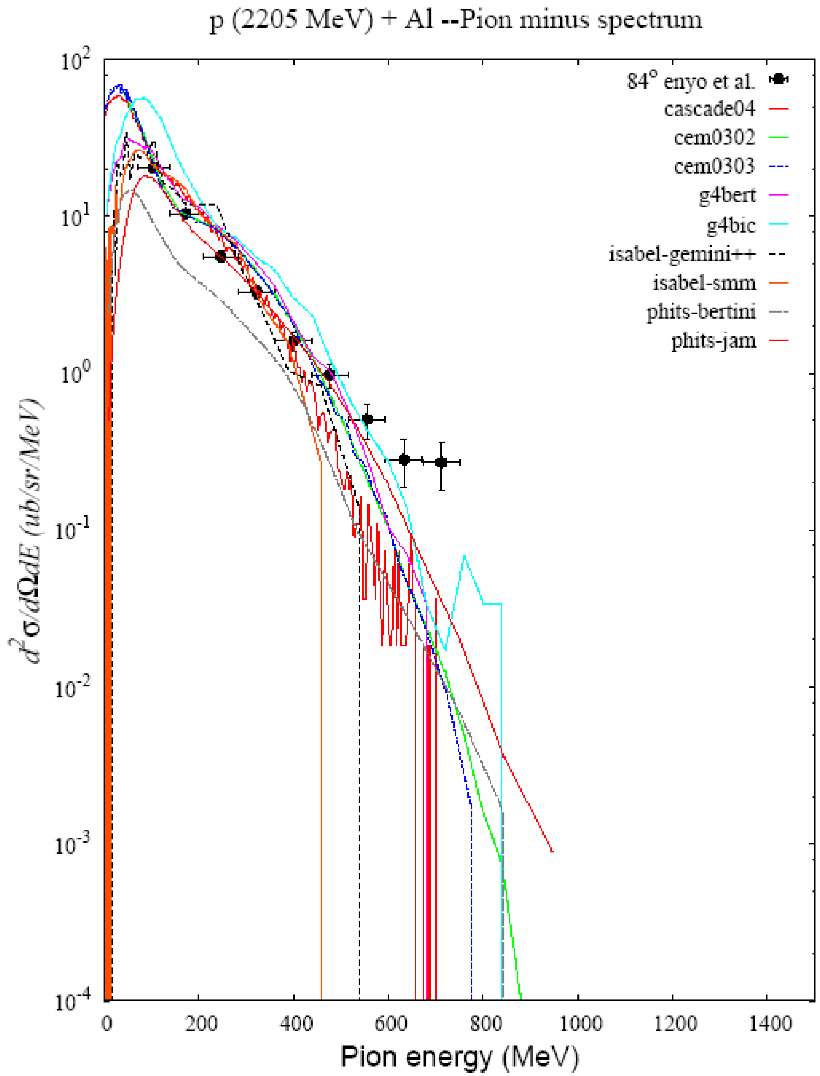



## Backward angle



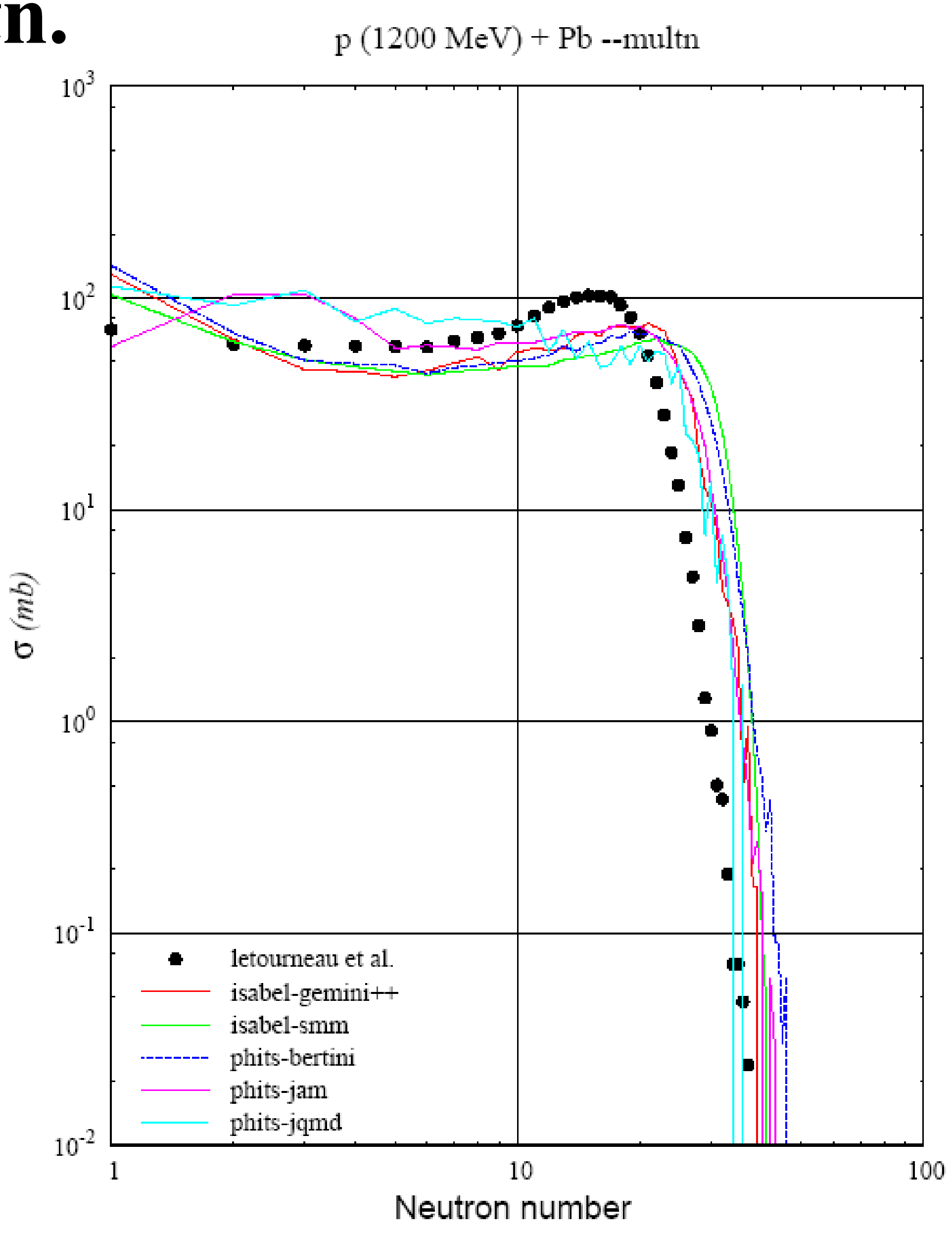
# Pion minus production



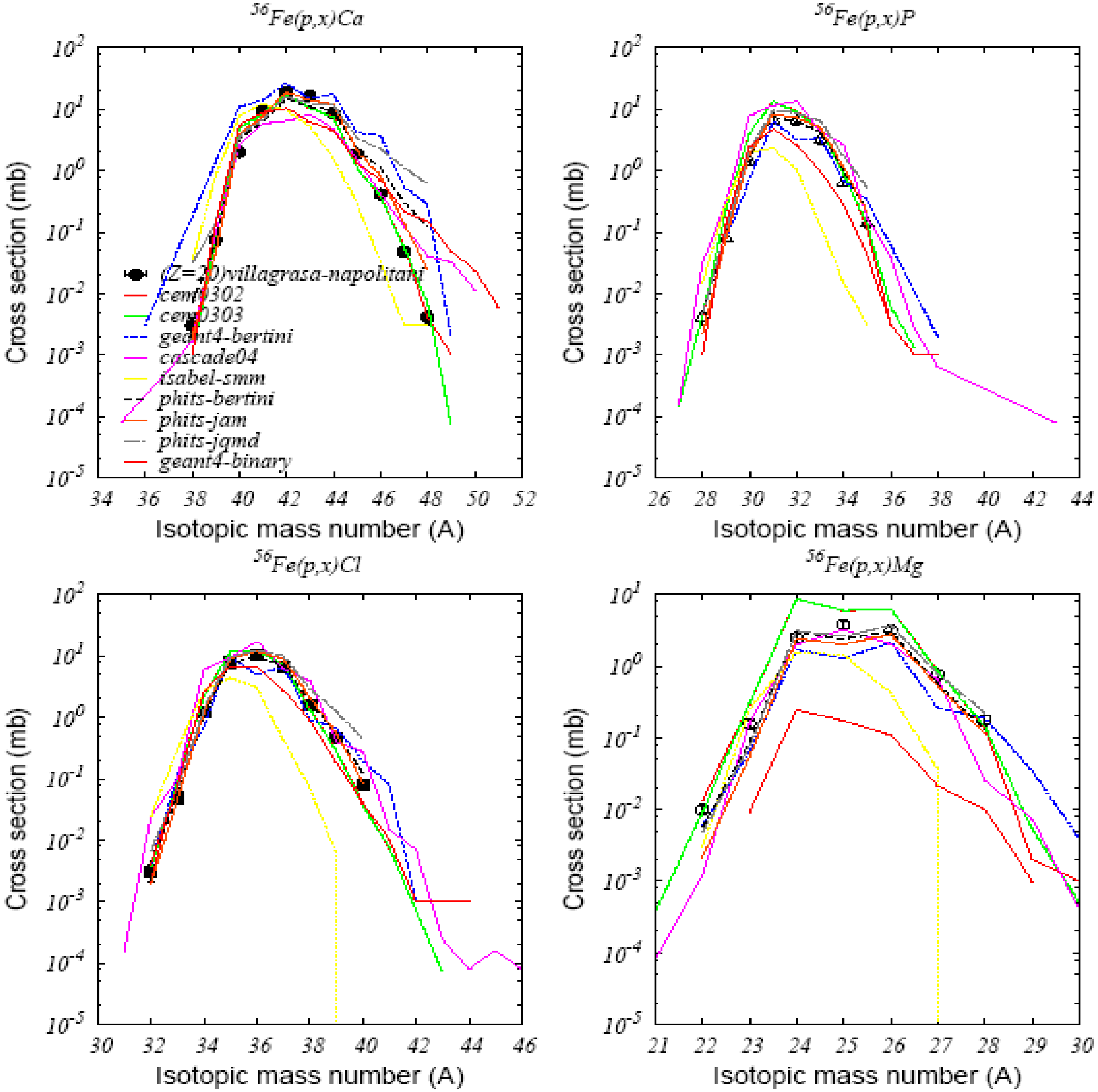



# Neutron multiplicity distn.

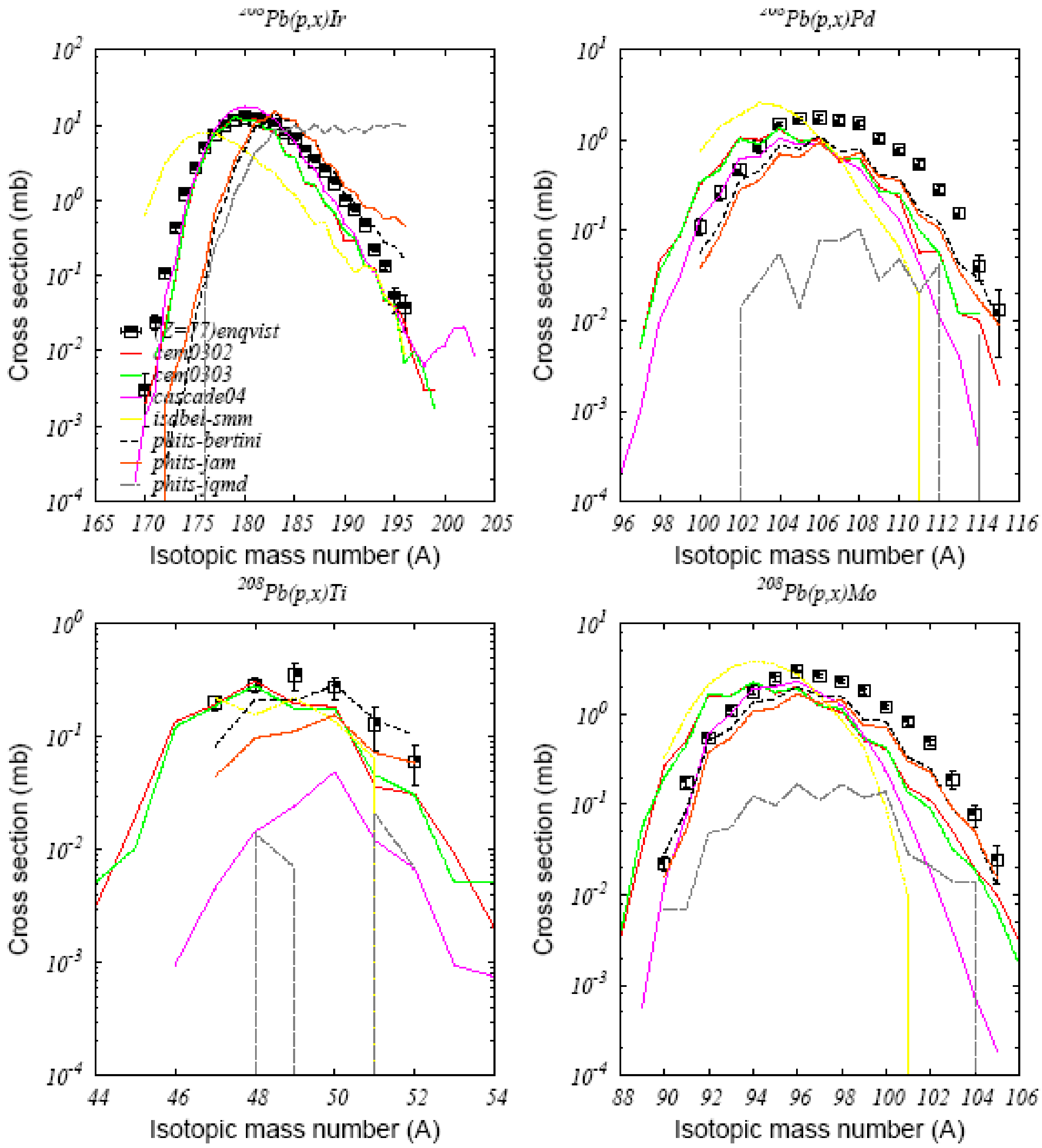
**Data received from only**
PHITS-jam,
PHITS-bertini,
PHITS-jqmd,
Isabel-smm,
Isabel-gemini models



# Isotopic distn. for Fe target



# Isotopic distn. for Pb target



# 6. Excitation function

# Excitation function

Independent cross section (nuclear reaction only)

$$A(t) = N_{\mathrm{T}} \sigma \Phi (1 - \exp(-\lambda t)), \quad 0 \leqslant t \leqslant t_{\mathrm{irr}}$$

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

$$A_{\mathrm{D}}(t) = N_{\mathrm{T}} \Phi \left( \begin{array}{l} \left( \sigma_{\mathrm{D}} + \sigma_{\mathrm{M}} \dfrac{\lambda_{\mathrm{M}}}{\lambda_{\mathrm{M}} - \lambda_{\mathrm{D}}} \right) (1 - \exp(-\lambda_{\mathrm{D}} t_{\mathrm{irr}})) \exp(-\lambda_{\mathrm{D}} t) \\ \quad + \sigma_{\mathrm{M}} \dfrac{\lambda_{\mathrm{D}}}{\lambda_{\mathrm{M}} - \lambda_{\mathrm{D}}} (1 - \exp(-\lambda_{\mathrm{M}} t_{\mathrm{irr}})) \exp(-\lambda_{\mathrm{M}} t) \end{array} \right)$$

$\sigma$ = ???

IF $\lambda_M >> \lambda_D$ → $\sigma_C = \left( \sigma_{\mathrm{D}} + \sigma_{\mathrm{M}} \dfrac{\lambda_{\mathrm{M}}}{\lambda_{\mathrm{M}} - \lambda_{\mathrm{D}}} \right)$

## Excitation function

- Half-lives / Branching ratios: decay data library of DCHAIN-SP (EAF-3.1, FENDL/D-1, ENSDF, …)

- $\lambda_M >> \lambda_D$ (???) → $T_M/T_D$ ratio can be changed

# Example

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

- 147 Sm
  - 147 Pm
    - 147 Nd
      - 147 Pr
        - 147 Ce
          - 147 La
          - 148 La
  - 147 Eu
    - 147 Gd
      - 147 Tb
        - 147 Dy
        - 147mDy
        - 148mHo
          - 148nHo
        - 151mHo
      - 147mTb
      - 151 Dy
        - 151 Ho
          - 151mEr
        - 151mHo
    - 151 Tb
      - 151mTb
      - 151 Dy
        - 151 Ho
          - 151mEr
        - 151mHo
  - 151 Gd
    - 151 Tb
      - 151mTb
      - 151 Dy
        - 151 Ho
          - 151mEr
        - 151mHo
    - 151mTb

## p(1400 MeV) + $^{54}Fe$ → $^{35}Cl$ + X

### Contribution to $\sigma_c$

35 Cl (1400. MeV)

| | | | |
|---|---|---|---|
| 0.7630 | | | |
| | 0.2251 | 0.9813 | |
| | | 0.0187 | 1.0000 |
| | | | 0.0000 1.0000 |
| | | | 0.0000 1.0000 |
| | 0.0119 | 1.0000 | |
| | | 0.0000 | 1.0000 |
| | 0.0000 | 1.0000 | |

= 1.000

= 1.000

### Progenitor Chain

35 Cl
35 S
35 P
35 Si
36 Si
35 Ar
36 Ca
36 K

nuclear reaction

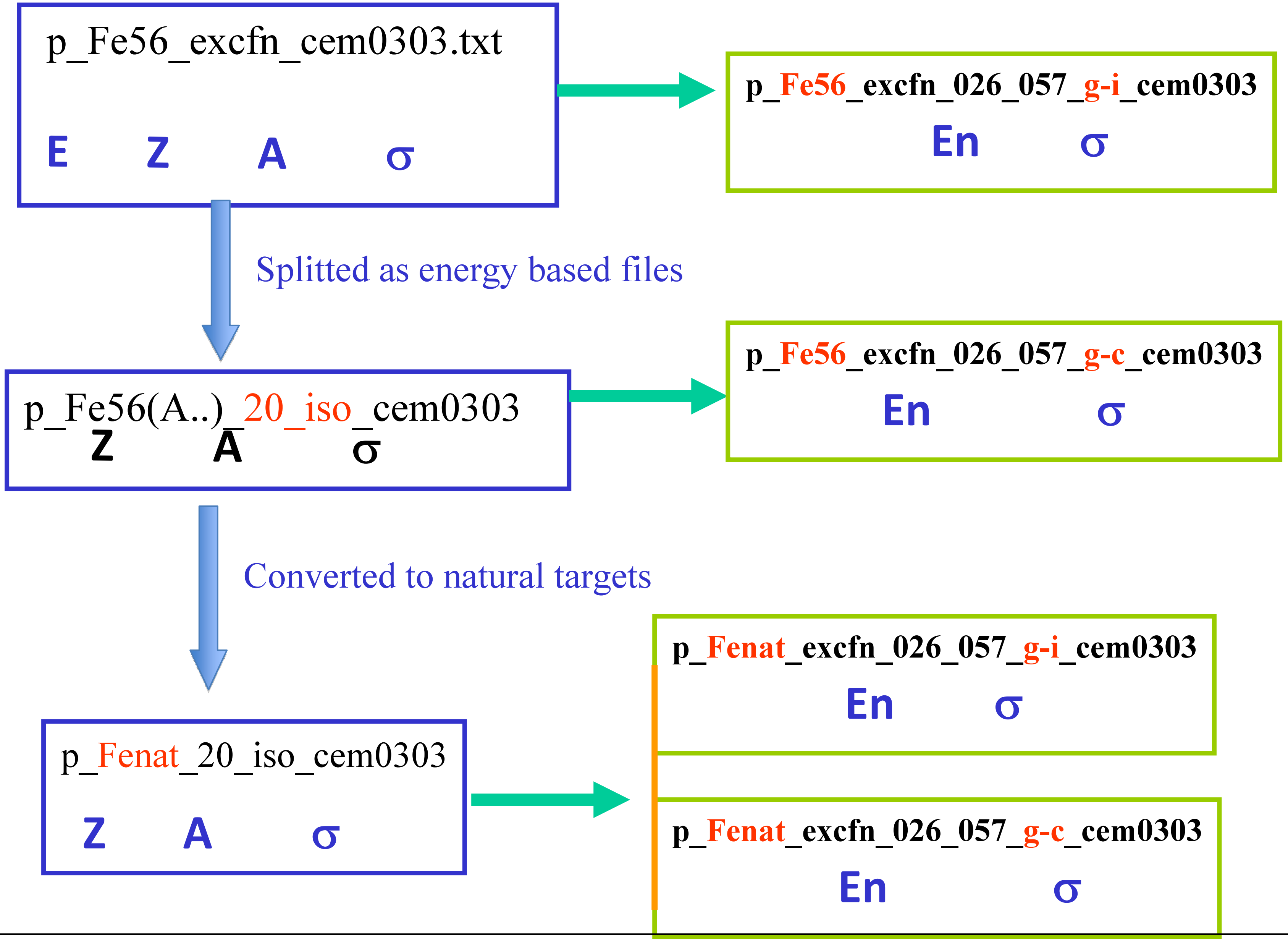
decay of precursor(s)

## Status of the excitation function data

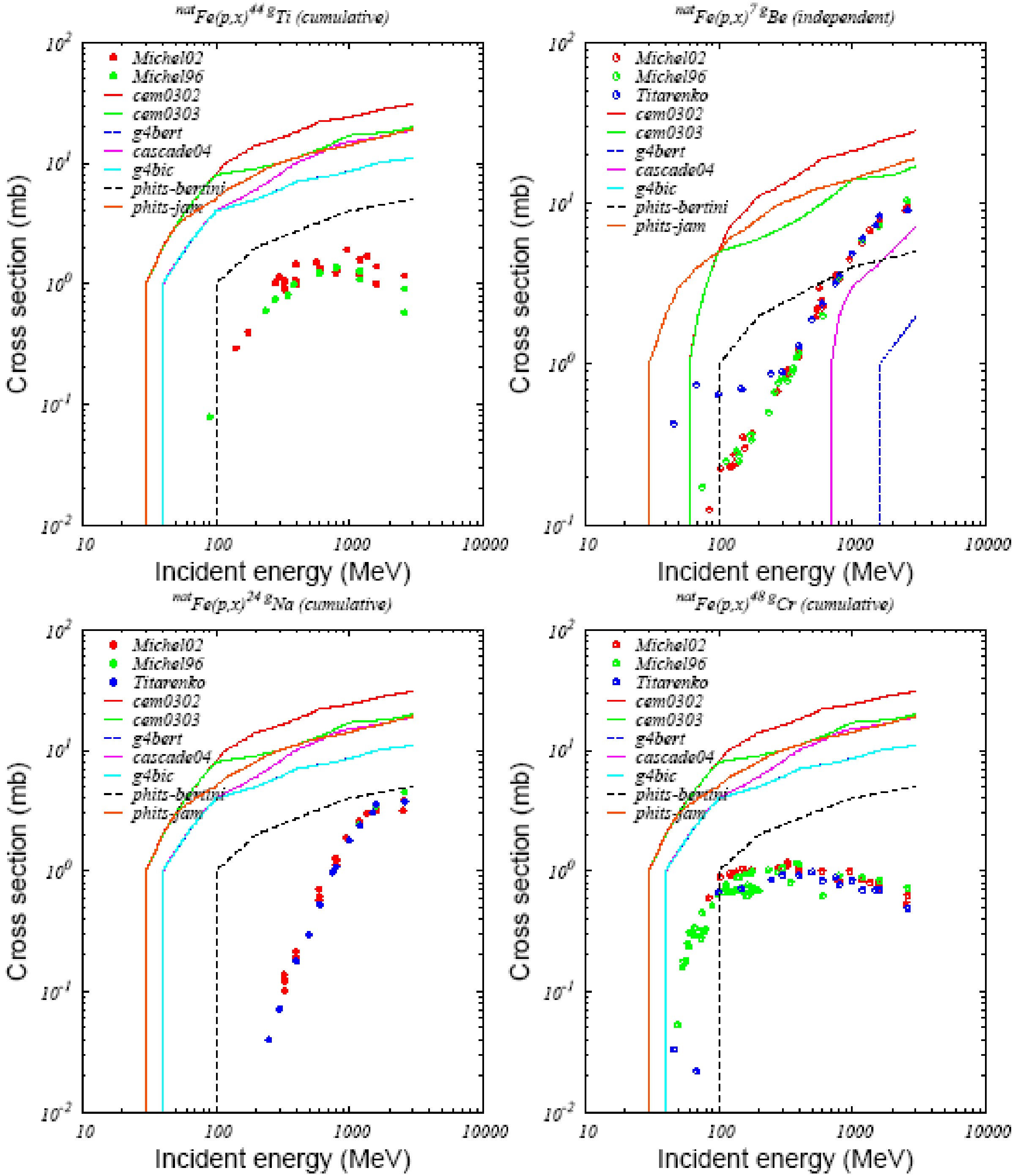
| Codes | Given data as |
|---|---|
| CEM0302 | p_Fe56_20_iso_cem03_02<br>**Z A σ dσ** |
| CEM0303 | p_Fe56_excfn_cem0303<br>**E Z A σ dσ** |
| Cascade04 | p_Fe56_20_iso_cascade04<br>**Z A σ dσ** |
| PHITS-jam*<br>PHITS-bertini* | p_Fe_50_iso_phits(JAM)<br>p_Pb_50_iso_phits(Bertini)<br>**Z A σ** |
| Geant4-binary<br>Geant4-bertini | p_Fenat_20_excfun_g4bic<br>p_Pbnat_20_excfun_g4bert<br>**Z A σ dσ** |

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

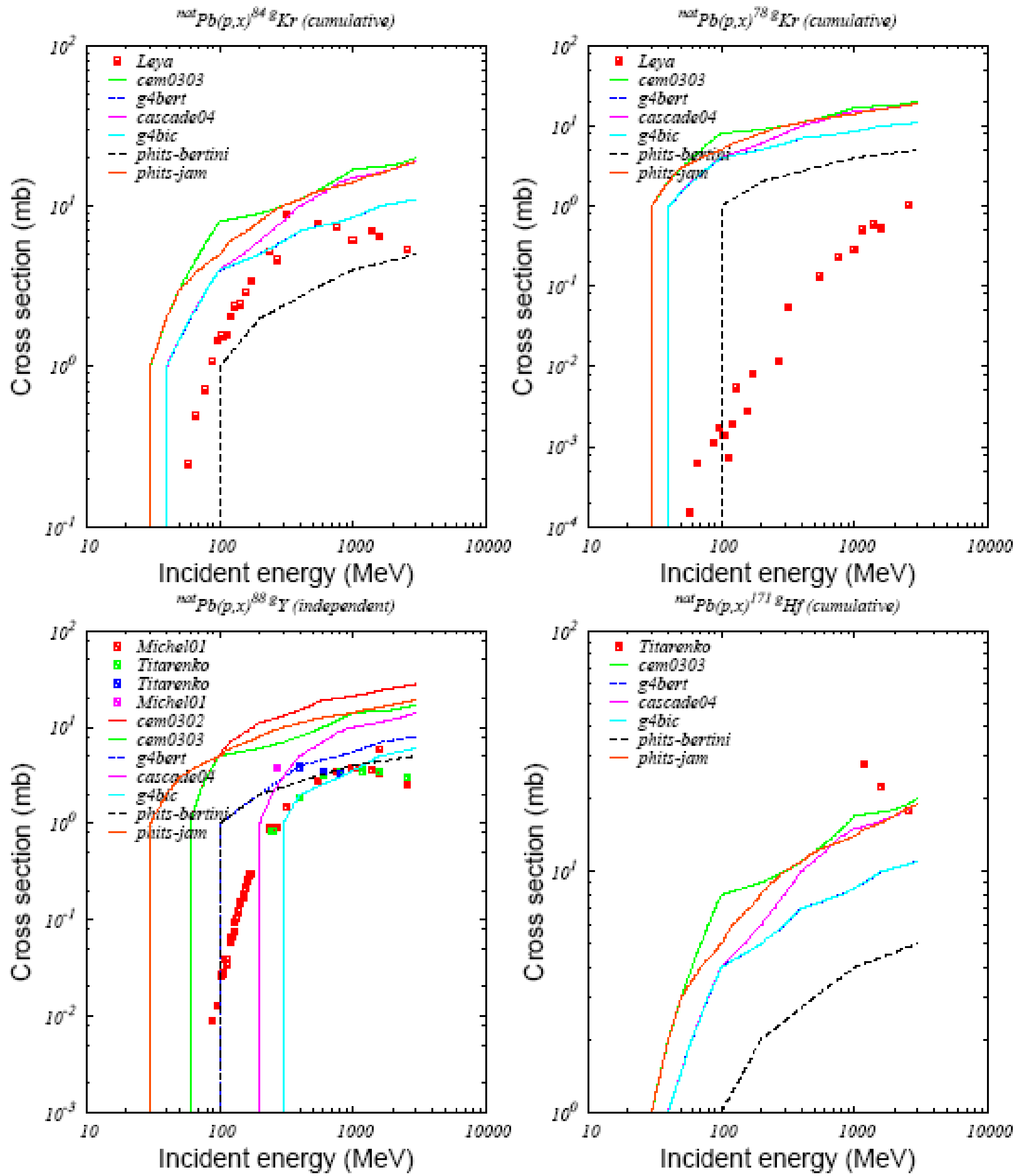
# Excitation function Data processing



# Excitation functior 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**