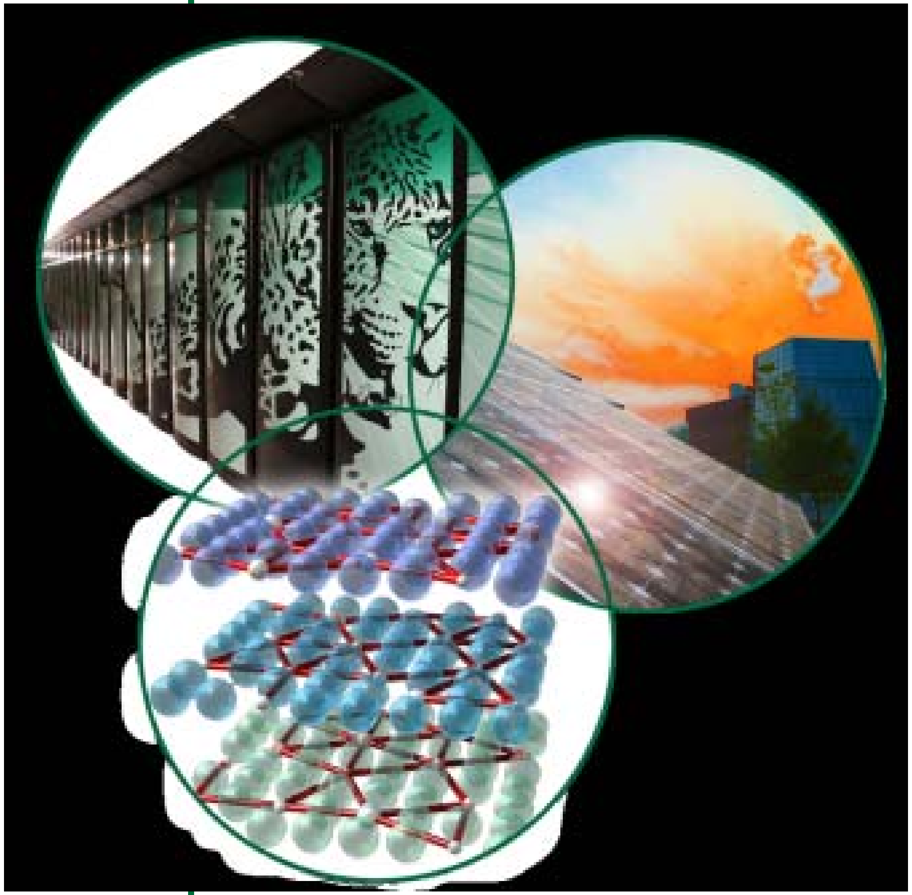
The MCNPX-Bertini-Dresner Results



Workshop on Spallation Model Benchmark

February 8-11, 2010

Franz Gallmeier

U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY

Outline

- MCNPX Bertini-Dresner Physics
- The Procedure of Calculations
- Neutron Results
- LCP results
- Residual and Excitation Function Results

MCNPX-Bertini-Dresner

- **Bertini space-like INC developed 1962-1971: MECC-1 to MECC-7 at ORNL**
  - **Physics described in**
    - **Bertini, Phys. Rev. C, Vol 6, No 2, p 631-659 (1973)**
    - **Bertini, Phys Rev. Vol 188, No 4, pp1711-1730 (1969)**
    - **Bertini, Phys. Rev. Vol 131, No 4, pp 1801-1821 (1963)**

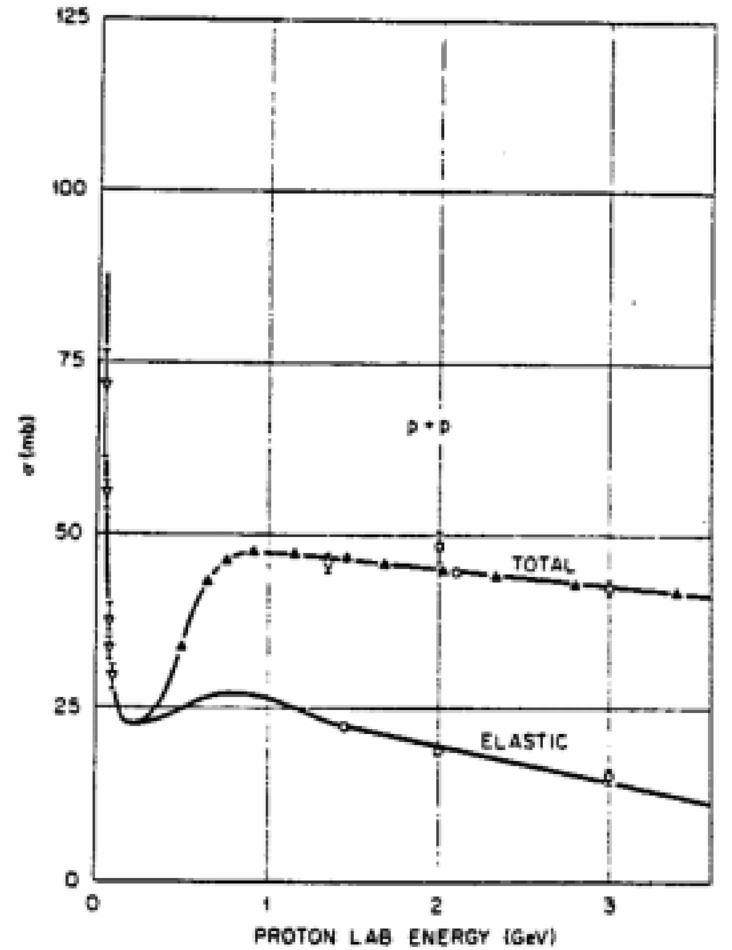


FIG. 1. Proton-proton total and elastic cross sections: ▲, D. V. Bugg *et al.* (see Ref. 15); ▽, U. E. Kruse *et al.* [quoted by F. F. Chen, C. P. Leavitt, and A. M. Shapiro Phys. Rev. 103, 211 (1956)]; □, T. Ferbel *et al.*, in *Proceedings of the 1962 International Conference on High-Energy Physics at CERN*, edited by J. Prentki (CERN, Geneva, 1962), p. 76; ○, S. P. Kruchinin *et al.*, Yadern. Fiz. 1, 317 (1965) [transl.: Soviet J. Nucl. Phys. 1, 225 (1965)].

Bertini Physics

- Spherical model of nucleus:
  - Three-region nuclear configuration with different densities of neutrons and protons where nuclear density reaches values of 0.9. 0.2 and 0.01 times central density based on data from Hofstadter
  - Binding energy of most loosely bound nucleons is7 MeV
  - Sternheimer-Lindenbaum isobar model for branching ratios and kinematics of pion-production
  - One and two pion production processes considered

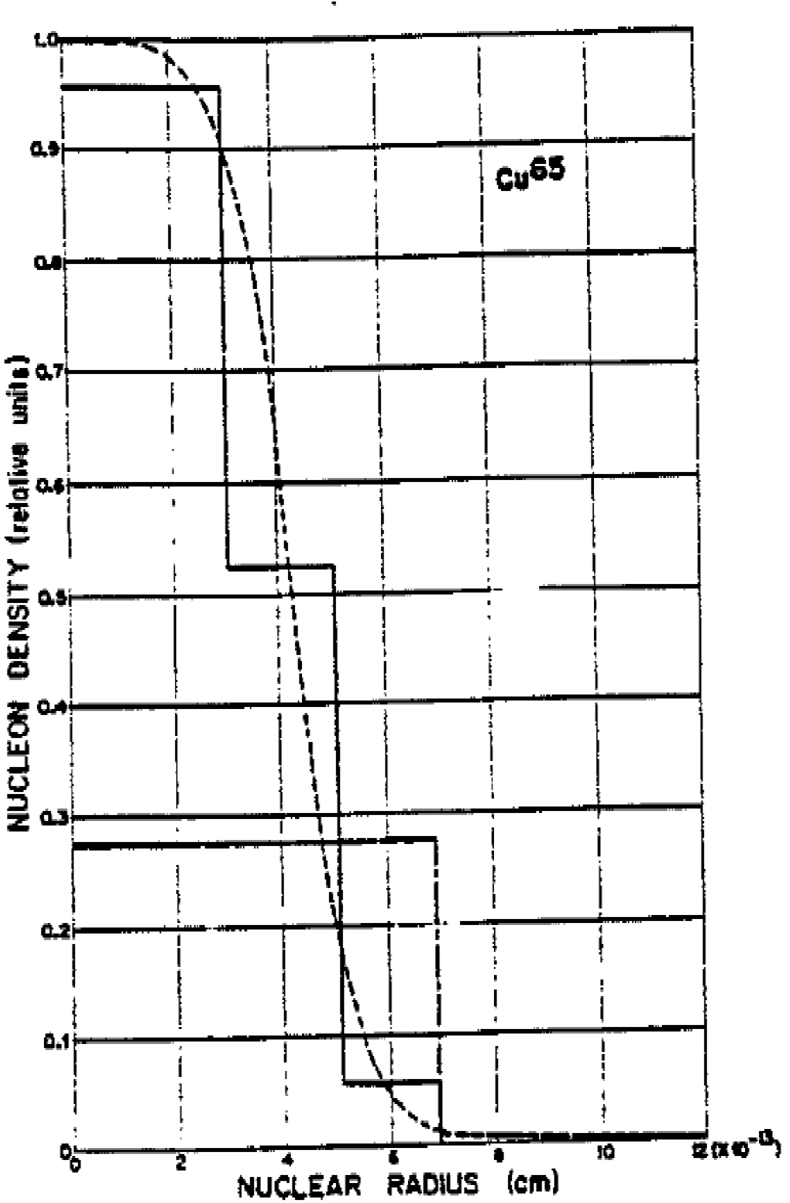


FIG. 1. A comparison of various nucleon-density distributions for nucleons inside the nucleus. Solid line, standard three-region configuration; long-dash—short-dash line, uniform distribution; dashed line, Hofstadter's curve (see Ref. 5).

Bertini Physics

- Emission of p, n, pi+, pi-, pi0
- Cascade termination if:
  - Either all cascade particles escaped
  - Energy dropped below one-half of Coulomb potential at nuclear surface
- Range of operation: incident nucleons 1-3500 MeV, incident pions 1-2500 MeV
- Claimed range of applicability: incident nucleons 100-2500 MeV, incident pions 100-1500 MeV

Dresner Physics

- **EVAP code developed by Dresner based on Weisskopf's evaporation theory and a Monte-Carlo code written by Dostrovsky:**
  - **Emission of neutrons and charged particles proton-Be10**

EVAP - A FORTRAN Program for Calculating the Evaporation of Various Particles from Excited Compound Nuclei

Lawrence Dresner

ORNL - TM - 196

COPY NO. - 1

DATE - April 11, 1962

- **EVAP2-4 modifications by M. Guthrie: updates of masses and binding energies; restrict emission to six particle types: n, p, d, t, He-3, α**
- **Prael modifications: level-density model replaced by Gilbert-Cameron-Cook-Ignatyuk**

Fermi-Breakup

- Replaces evaporation for light residuals with A<17
- Based on prescription of Epherre, extended to
  - fragmentation into 7 pieces
  - intermediate unstable states possible
  - two-body fragmentation with Coulomb barrier, and parity conservation
- Here restricted to two- and three-body breakups

MPM Pre-equilibrium Model

- **Multi-step preequilibrium exciton model MPM (Prael et al)**
- **Emission of n, p, d, t, He-3, α**
- **Inverse reaction cross sections by a parameterization of Chatterjee**
- **Preequilibrium starts after termination of INC with a configuration of one particle-hole pair beyond the minimum particle-hole configuration as allowed by the outcome of INC**
- **Preequilibrium terminates upon reaching an equilibrium exciton number**

ORNL Fission model by J. Barish and F. S. Alsmiller (1980):

- **Based on statistical theory by P. Fong**
- **Phenomenological model based on Blatt Weisskopf level densities with a-factors based on LeCourtier**
- **Fission fragment distribution and energy distributions by experimental data from Epperson** *"Systematics of Mass Yield Distributions for Nuclear Fission of Neptunium" Dissertation, Dept. of Physics, Duke University, 1978.*
- **Covers only fission of actinide targets**

RAL Fission Model by F. Atchison(1980):

- **Phenomenological model with fission probability parameterized in charge number and energy for actinides, and fitted polynomials of the level density parameters for fission and neutron emission and fission barriers in Z^2/A.**
- **Mass and charge of fission products from phenomenological data and systematics.**
- **Fission allowed for targets with Z>70**

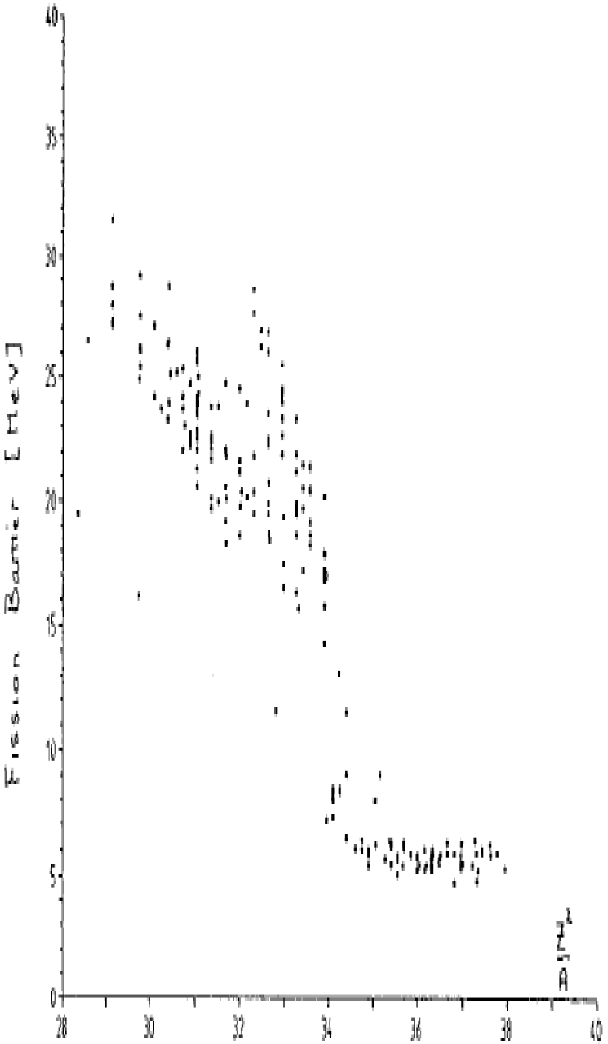


Figure 2: Measured fission barriers as a function of Z^2/A. The data comes from Dahlinger et al.[16]

Gamma-deexcitation

- **Gamma de-excitation for residuals resulting from evaporation/fission stage. Gamma de-excitation does not compete with evaporation.**
- **Gamma cascading using isotopic tabulated discrete energy levels from the RIPL library and continuum states with level densities given by the Gilbert-Cameron formula.**
- **Gamma de-excitation stops if a meta-stable state with a half-life of greater than 1 ms or the ground state is reached.**

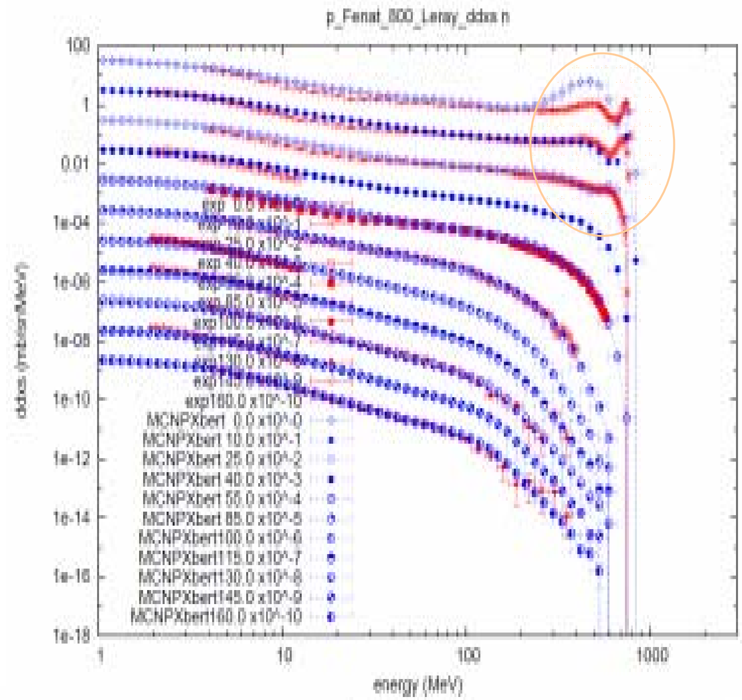
Procedure of Calculations

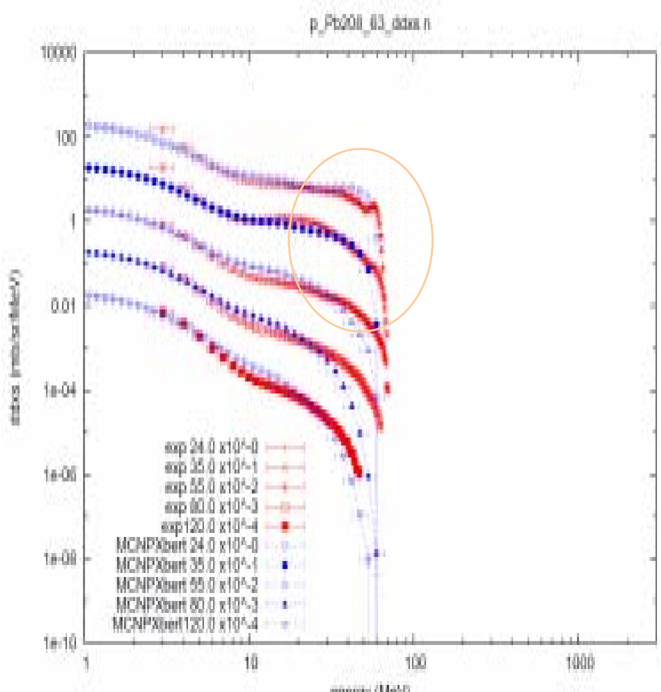
- **MCNPX_2.6.0 used for calculations**
- **Used the thin-target mode**
- **Switched off tabular data mode**
- **Used current tallies for double-differential emission yields**
- **Used isotope production tally for residuals (saved postprocessing of history tape)**
- **Normalized to empirical inelastic cross sections being used in MCNPX**
- **Post-processing scripts applied for normalization, writing results files and producing plots.**

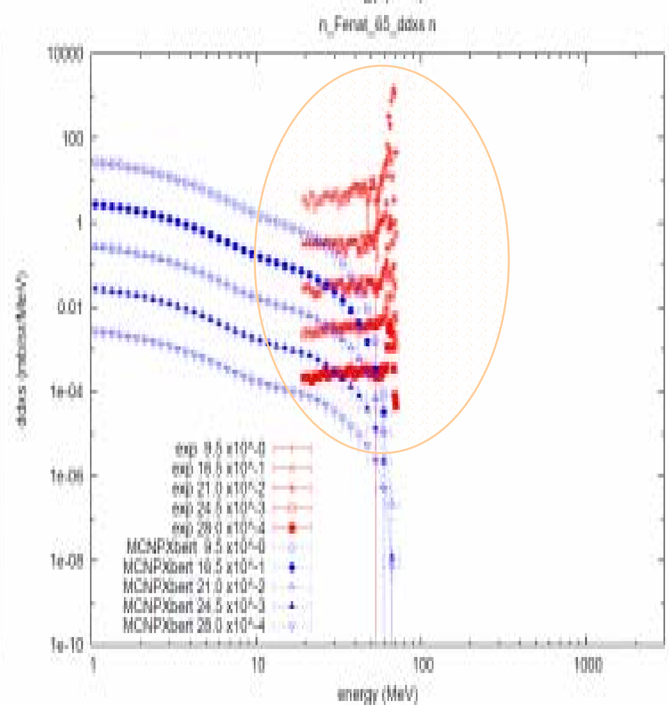
DDXS Data on the IAEA-webpage are not correctly normalized

Neutron Data

- **Neutron results are fairly good**
- **Deficits in forward direction at high E are probably caused by missing out on peripheral collisions due to using only three density zones**

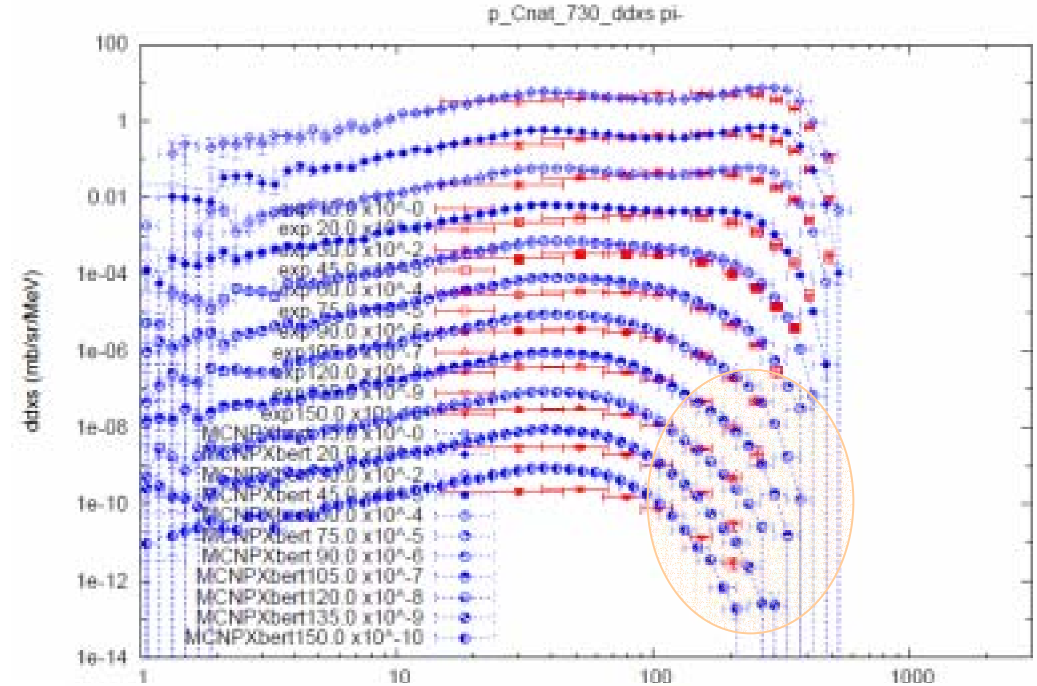


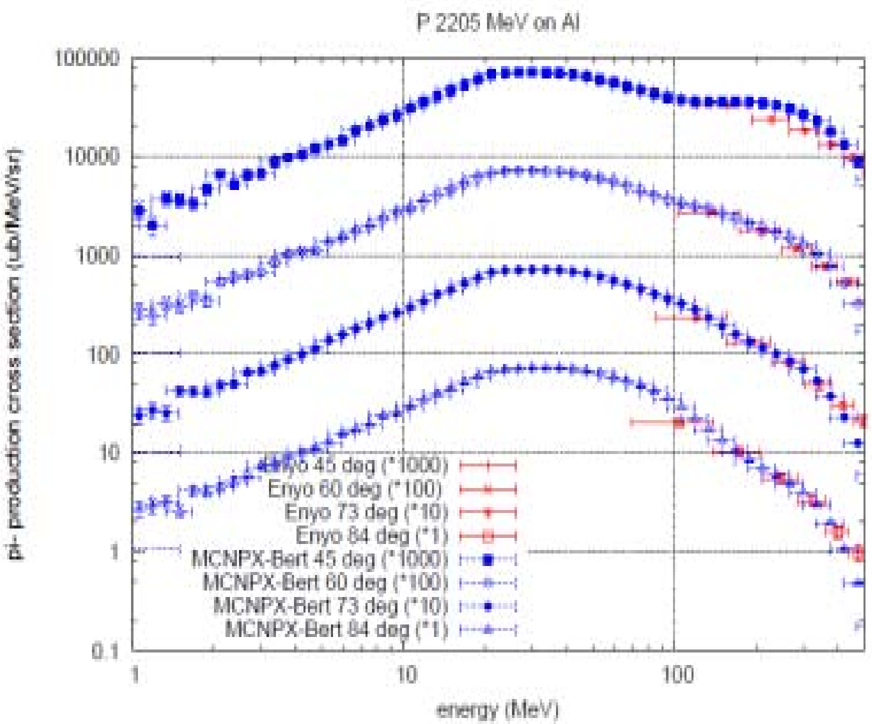


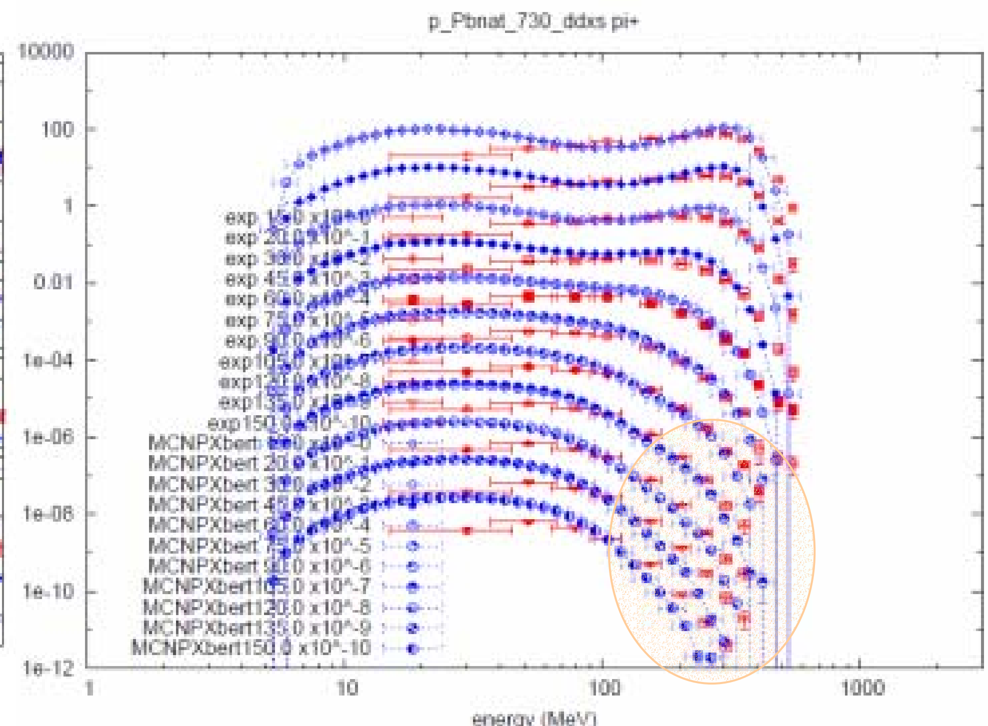


Pion results

- **Pion production looks good**
- **find larger deviation in high-E backward emission**

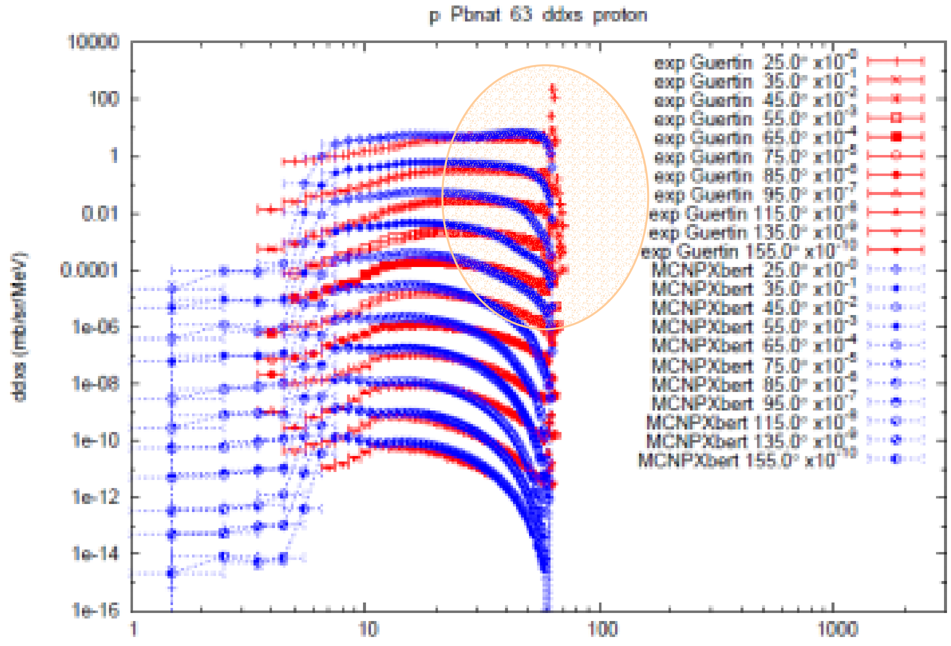


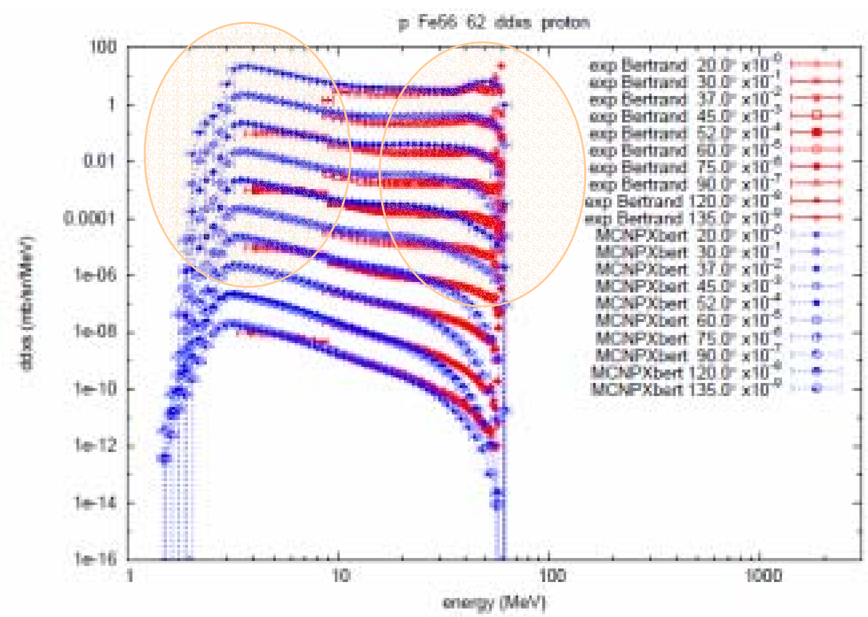


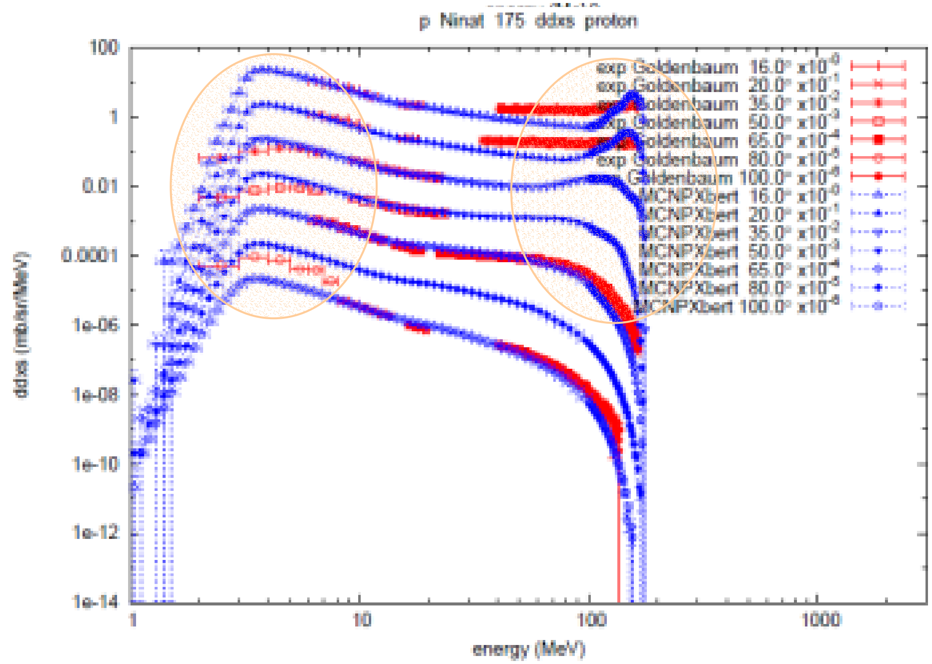


Protons low incident energy:

- **Quasielastic peak badly described**
- **Evaporation too high**

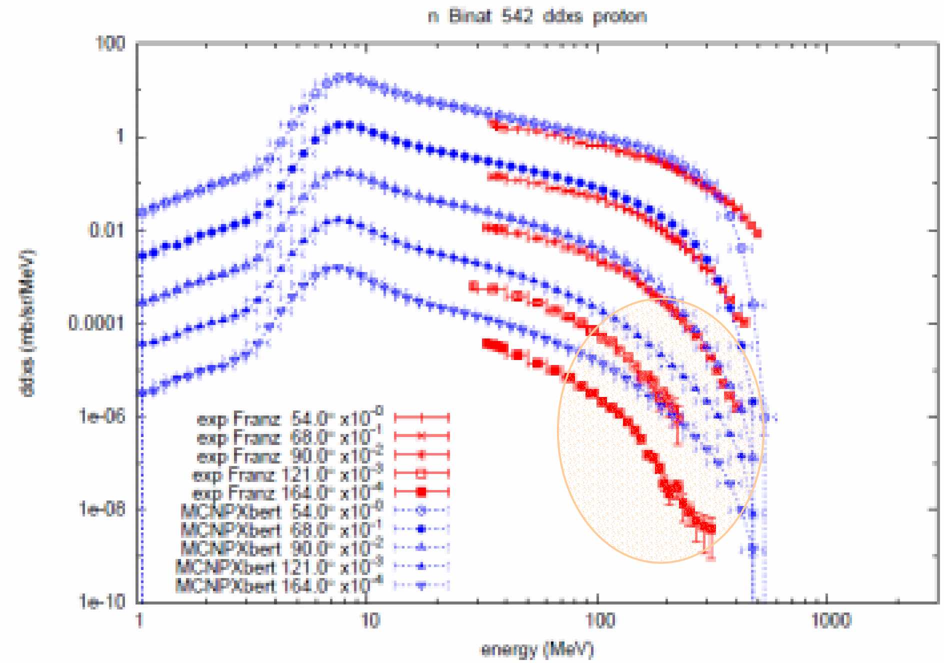


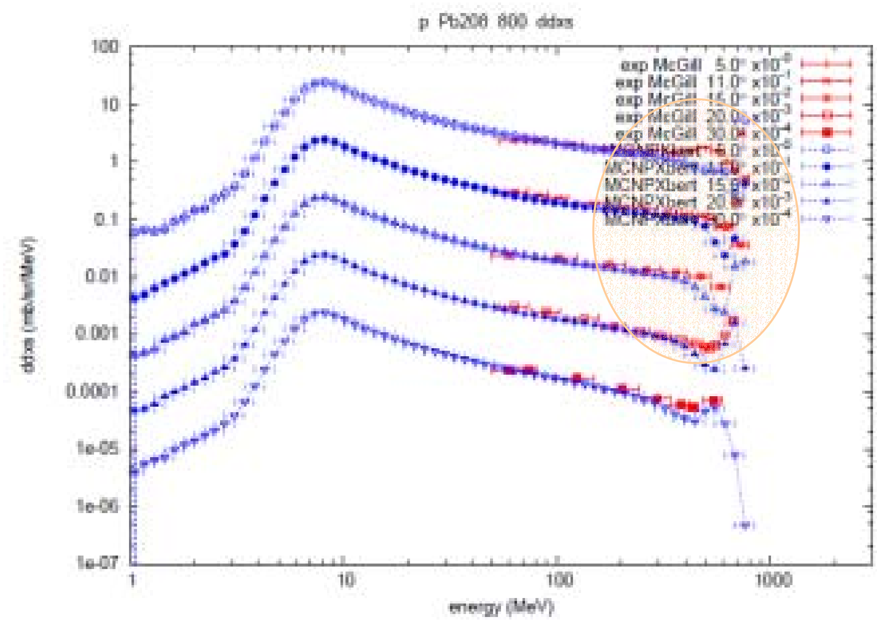




Protons intermediate incident energy:

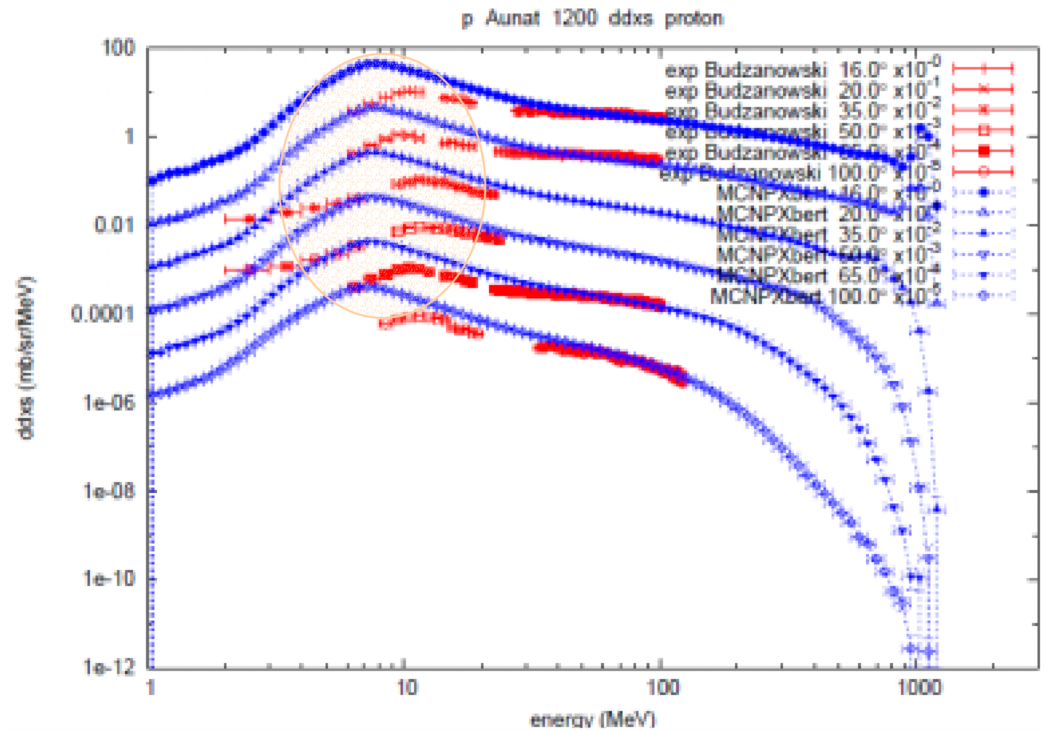
- **still problems at high E at forward angles**
- **also overestimation in backward direction**

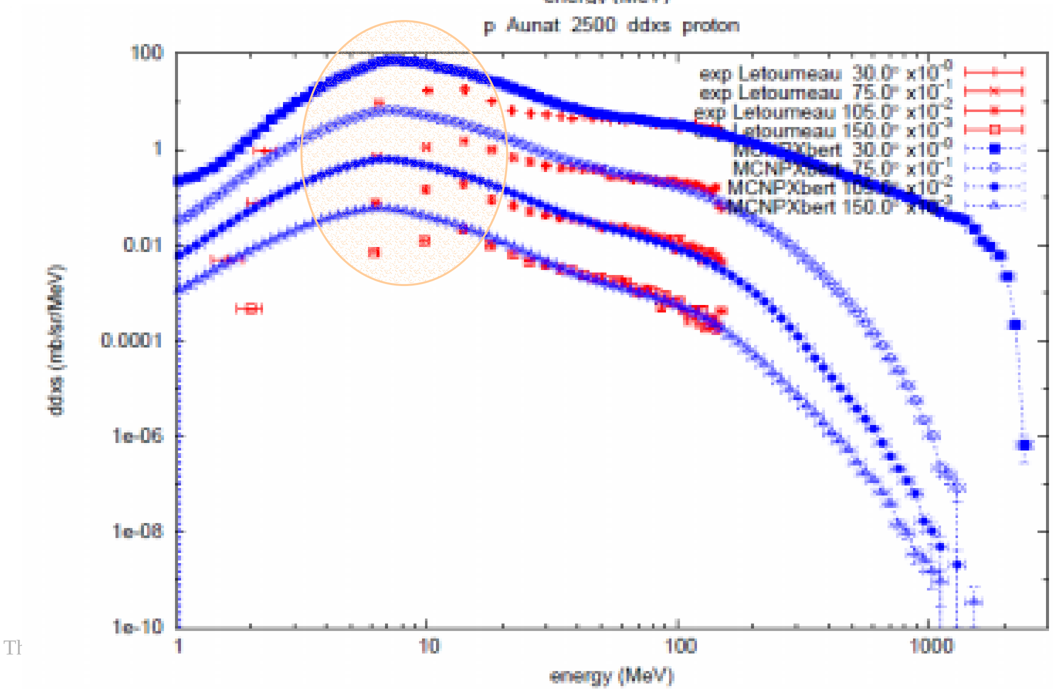




Protons high incident E heavy target mass

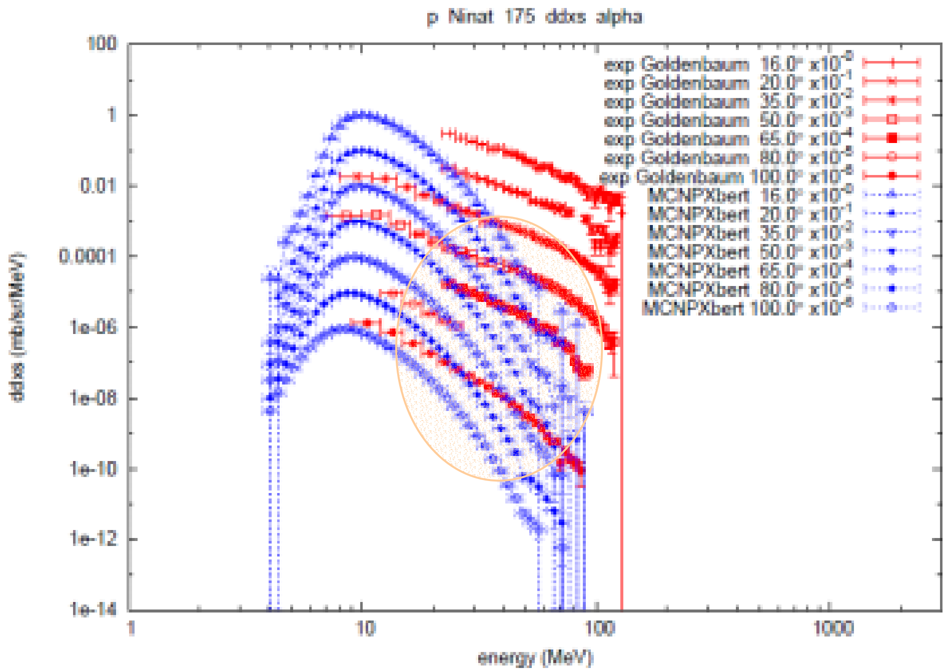
- **Evaporation**
  - **Peak at 7 MeV rather than 10 MeV**
  - **overestimated?**
- **Pre-equilibrium ok**

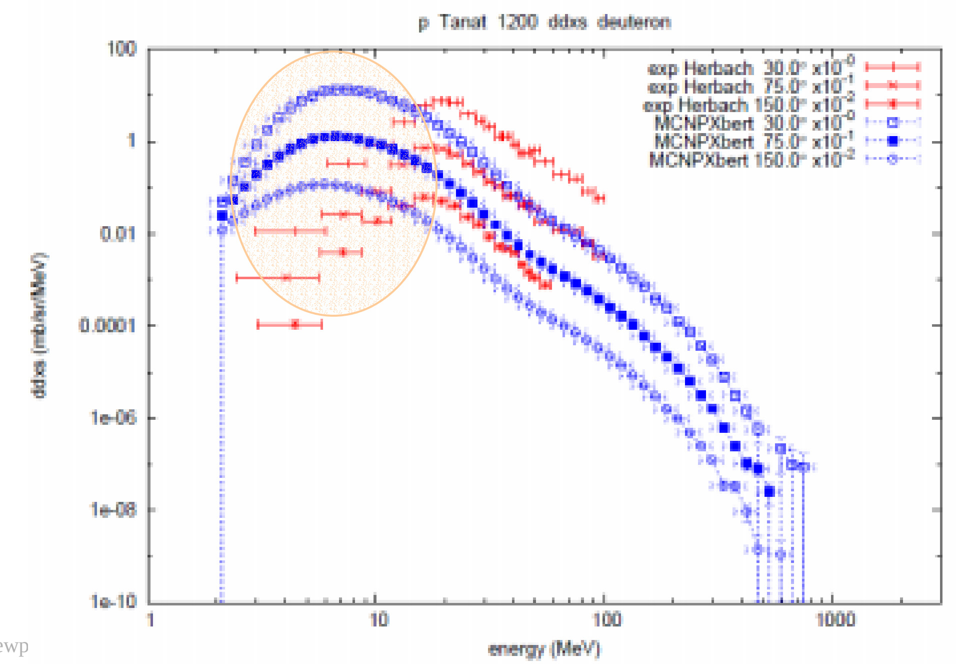




Higher-mass Charged particles

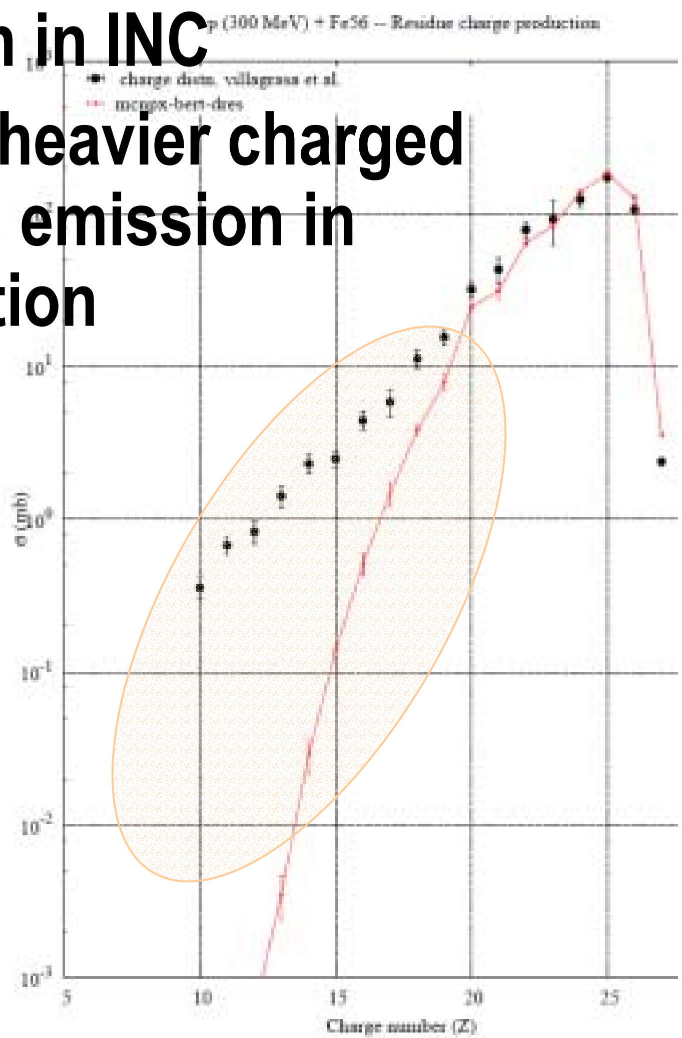
- **Composite particle emission missing in INC**
- **Pre-equilibrium emission underpredicted**
- **Evaporation overpredicted**

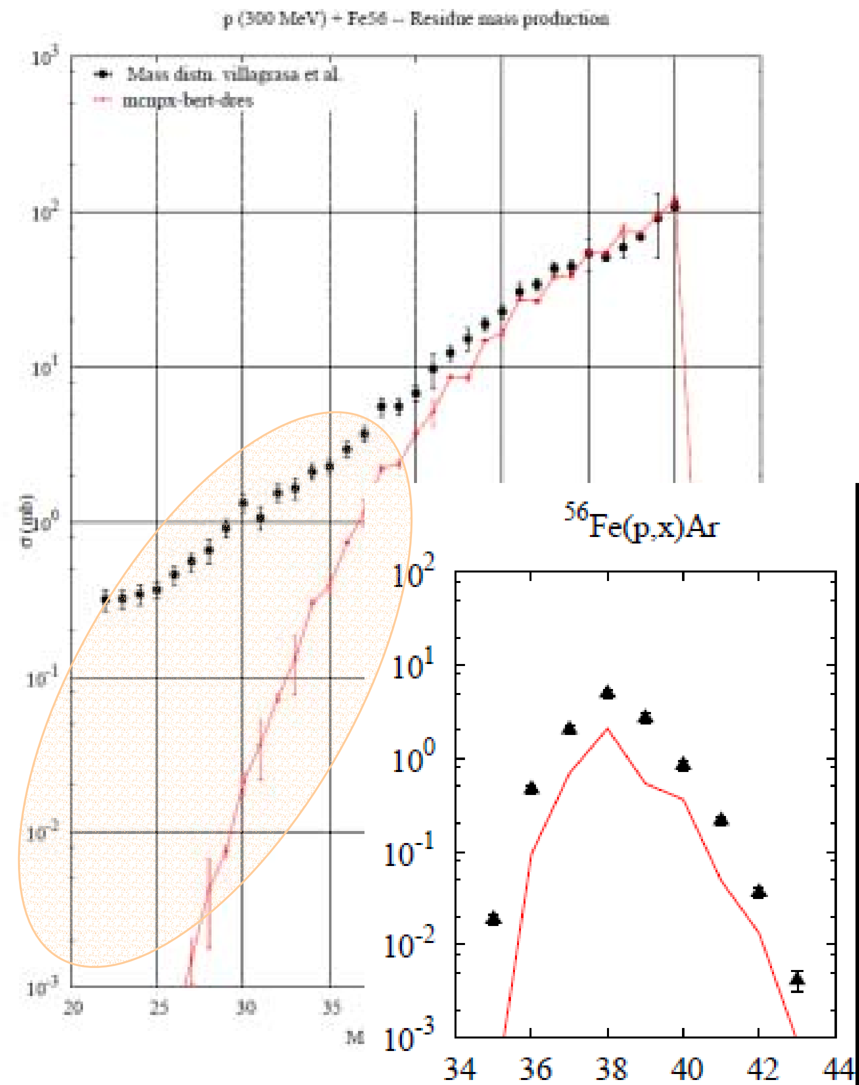




Residuals from Fe targets 300 MeV

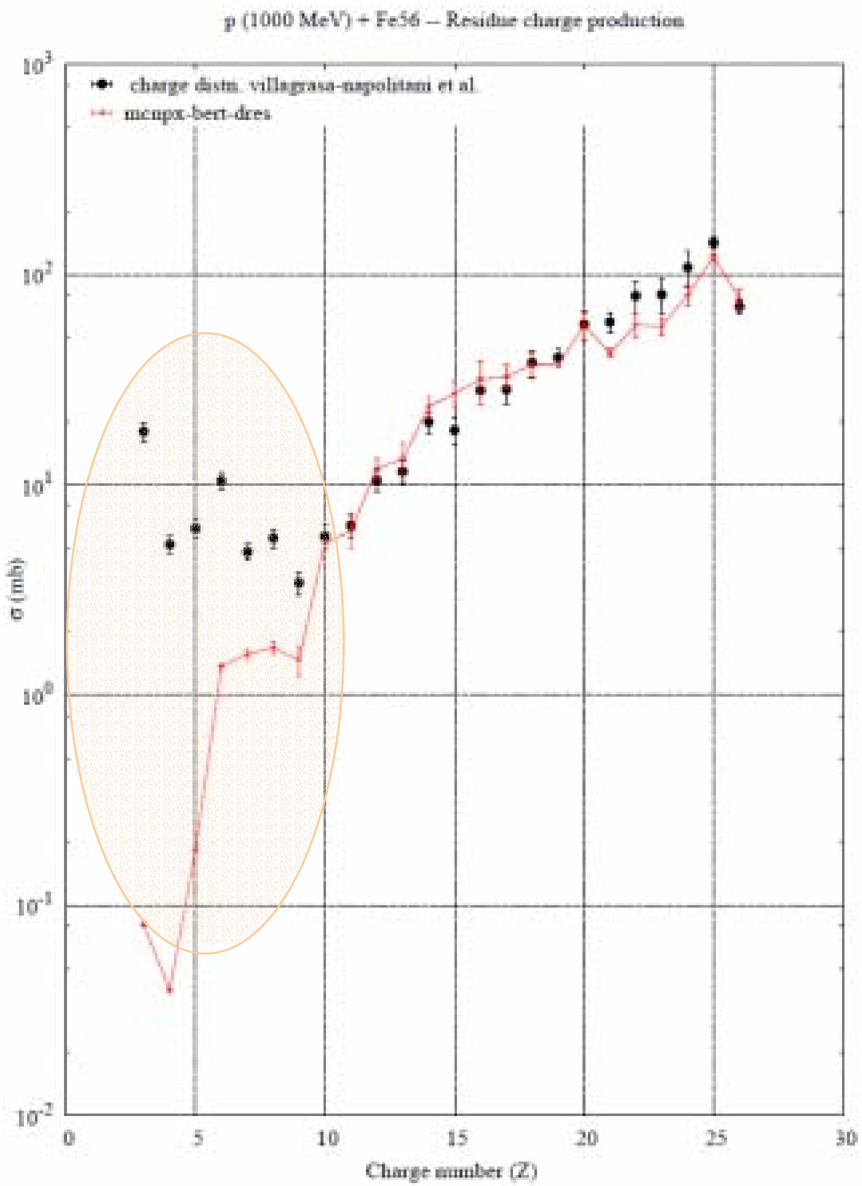
- **Not enough emission**
- **Missing composite particle emission in INC**
- **Missing heavier charged particles emission in evaporation**



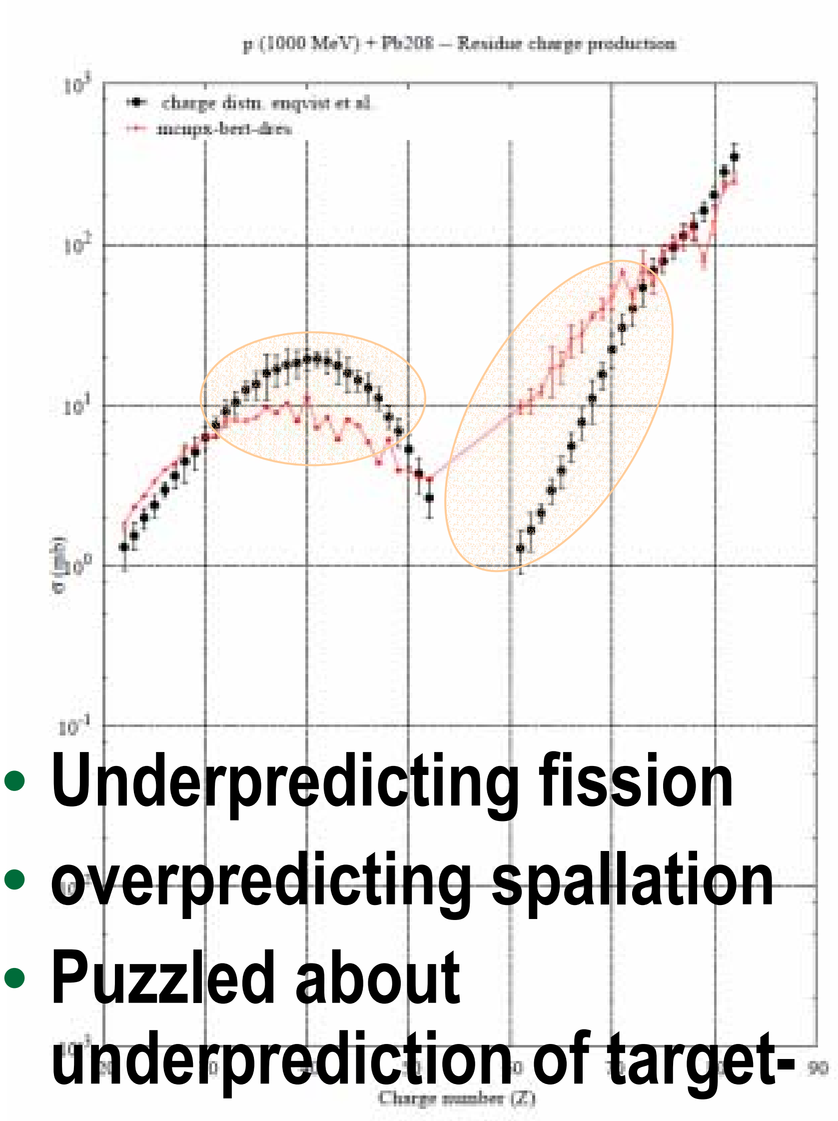


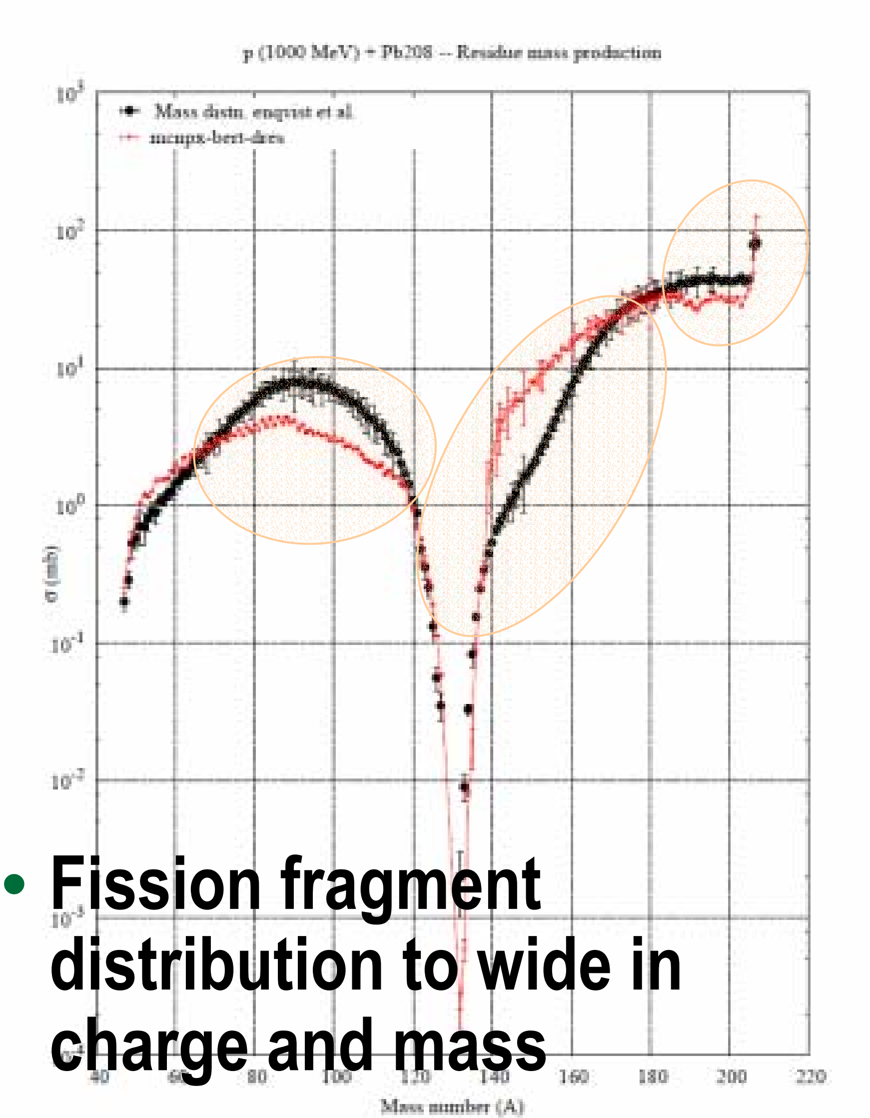
Residuals from Fe targets 1000 MeV

- **Missing heavy light charged particles emission in evaporation**



Residuals lead (with RAL fission model)

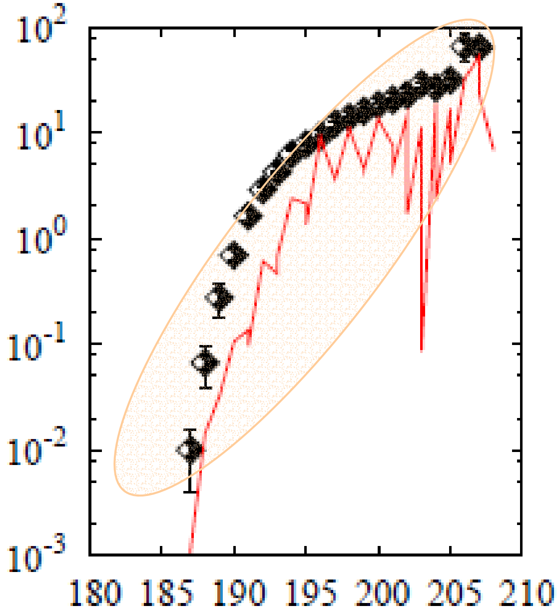


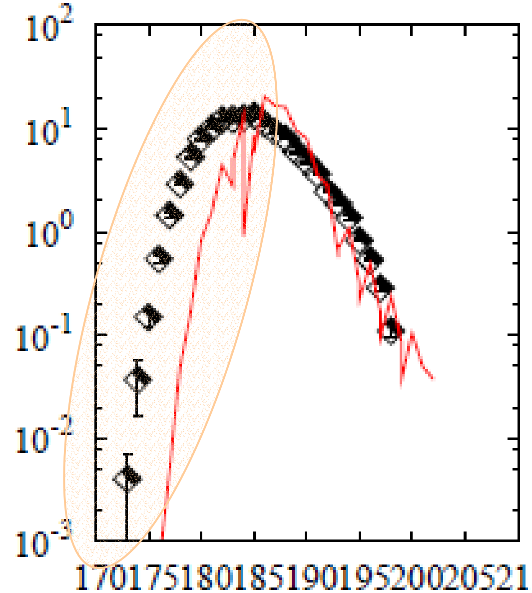


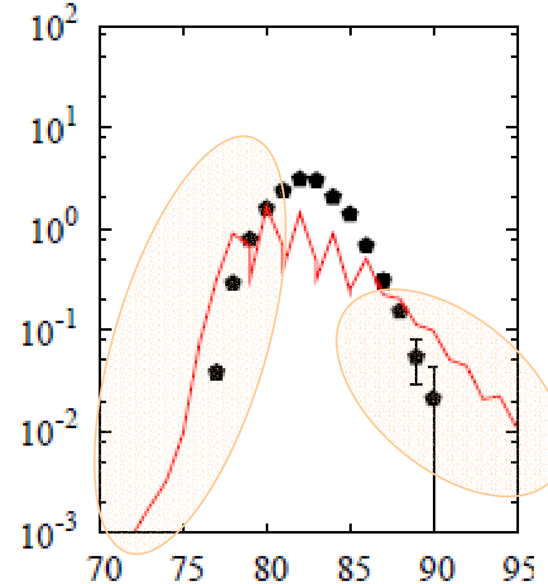
- **Underpredicting fission**
- **overpredicting spallation**
- **Puzzled about underprediction of target-near masses**

- **Fission fragment distribution to wide in charge and mass**

Residuals lead (cont)





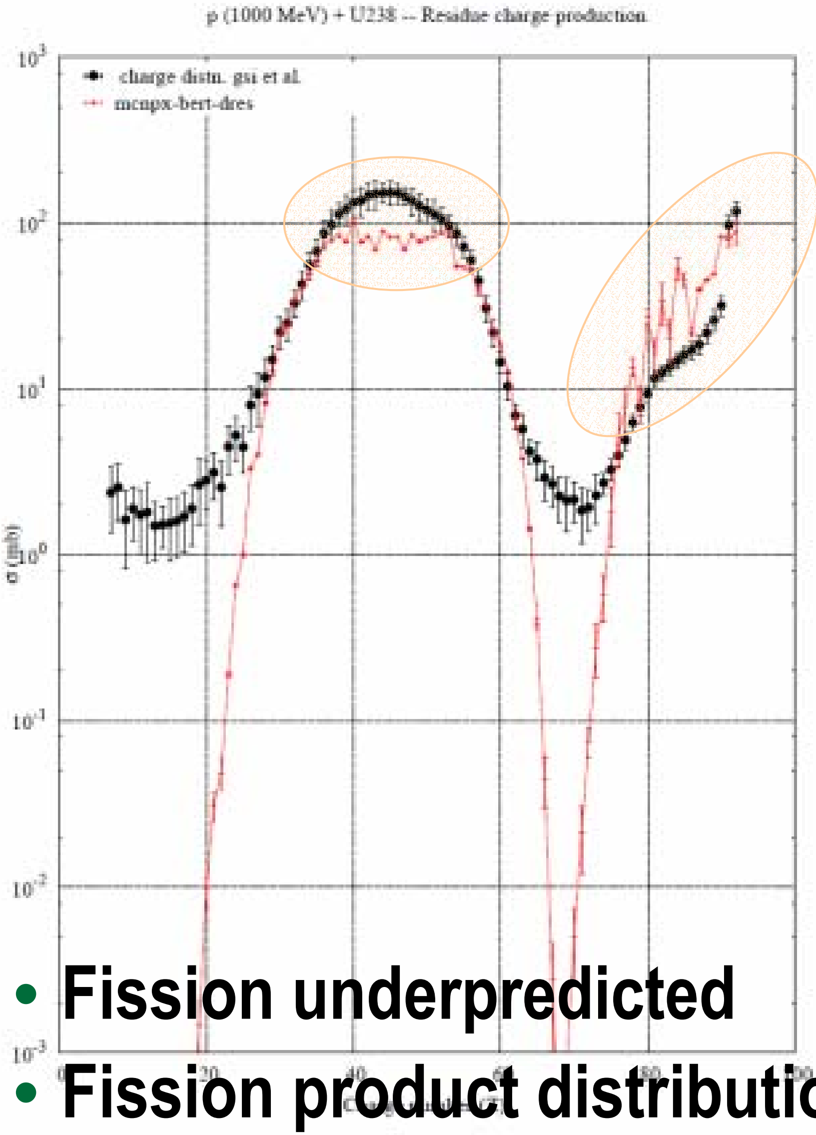


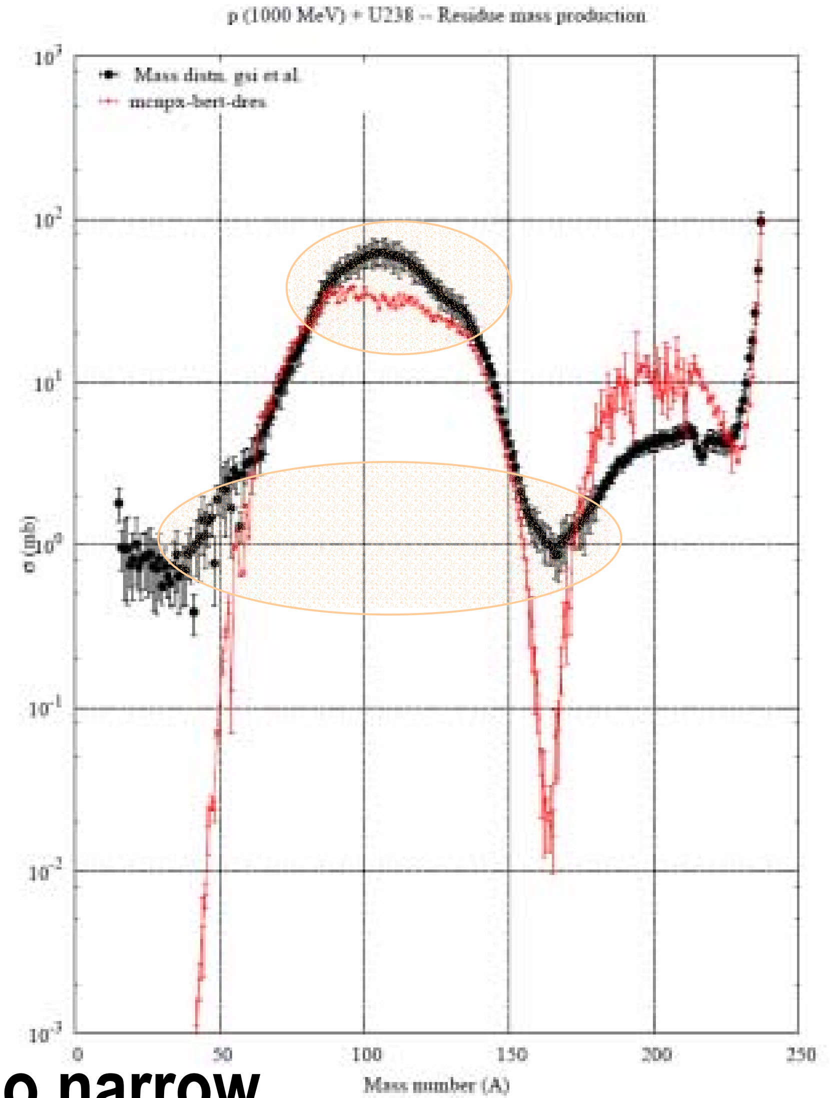
- **Overpredict proton emission**
- **Over-emphasizes shell effects**

- **Neutron poor wing missed**

- **Fission product mass distribution too wide**

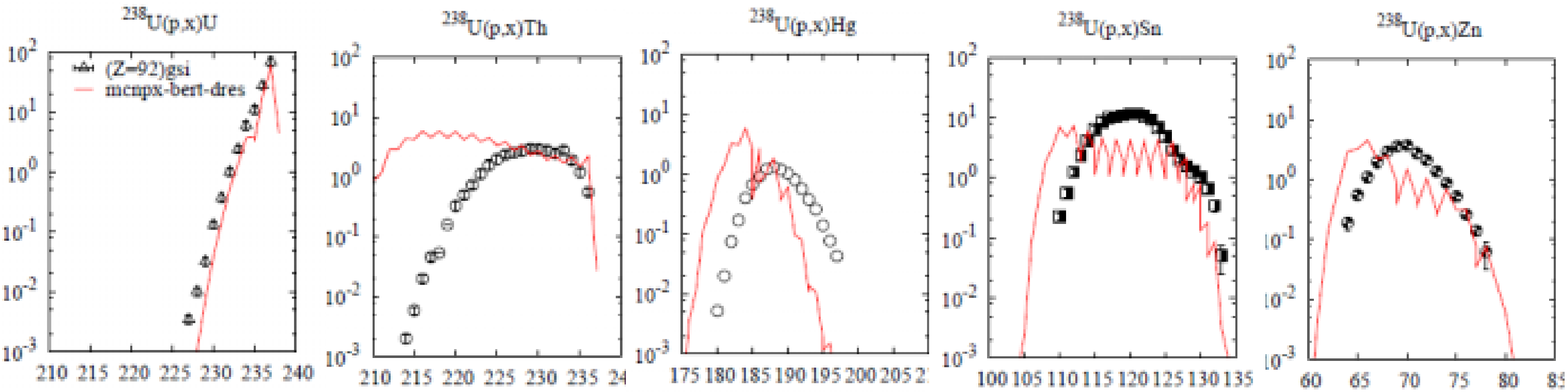
Residuals U238 (with ORNL fission model)





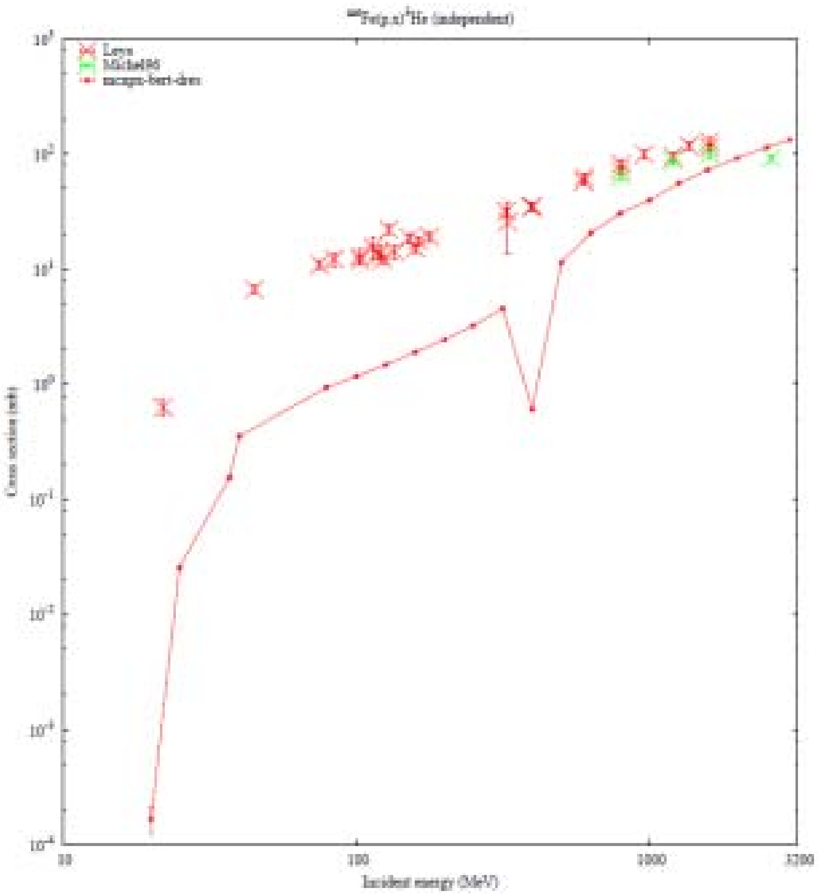
- **Fission underpredicted**
- **Fission product distribution too narrow**

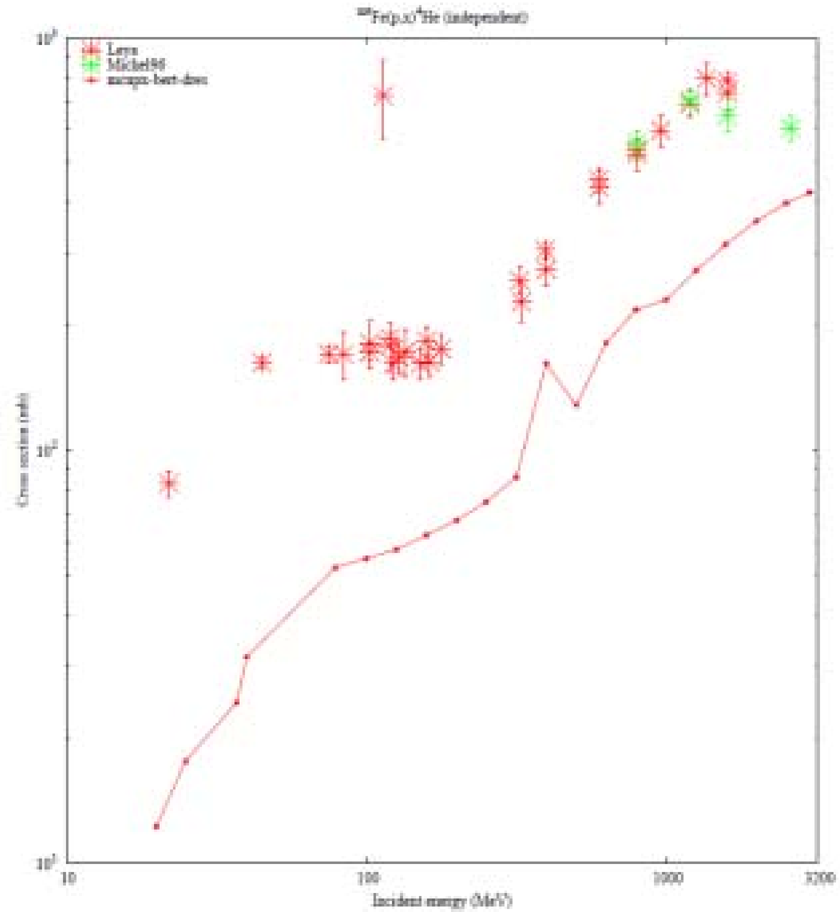
Residuals U238 (cont.)



- U isotopes slightly underestimated
- Spallation product masses overpredict neutron-poor wing
- Fission product distributions
  - too wide
  - flattened peak
  - Show strong shell effects

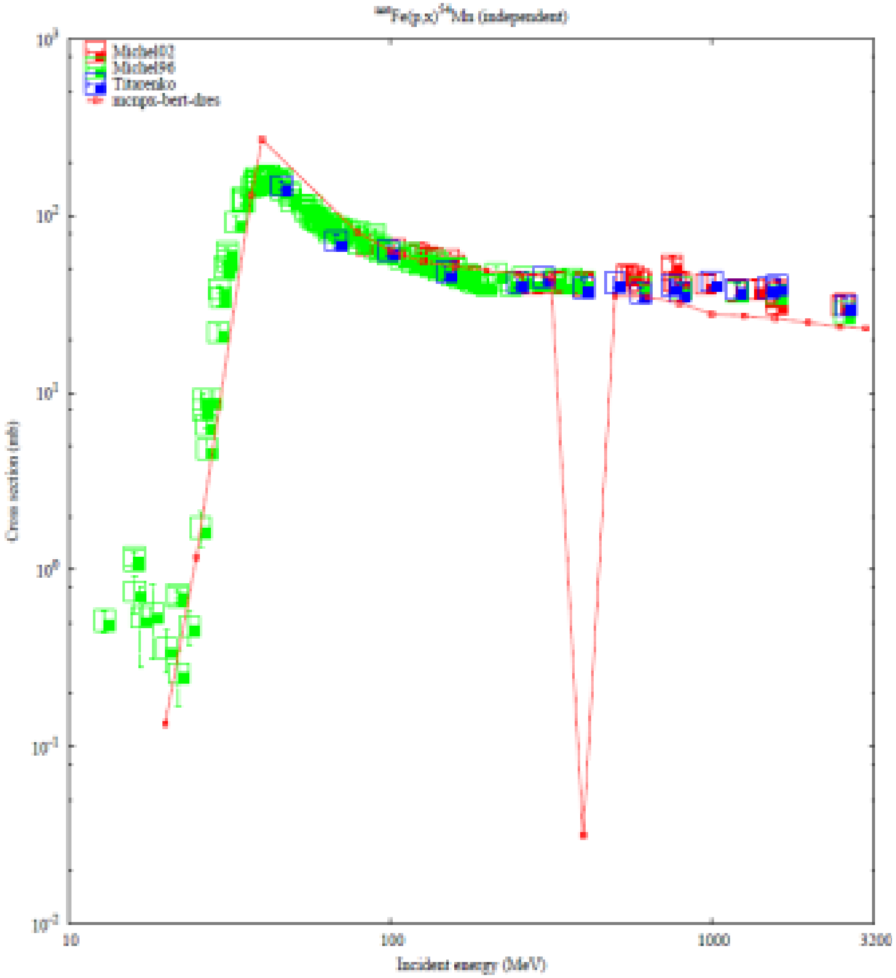
Excitation Functions Fe-nat

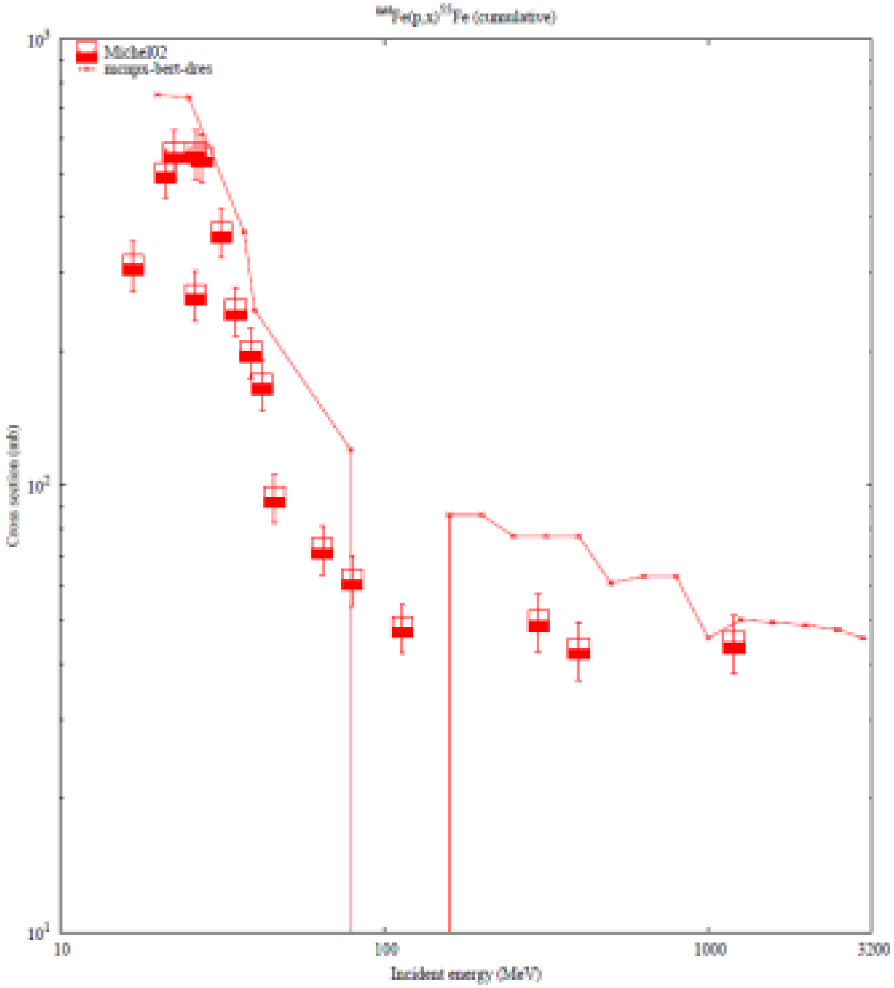




- **Underpredict He production (no complex particle emission in INC)**

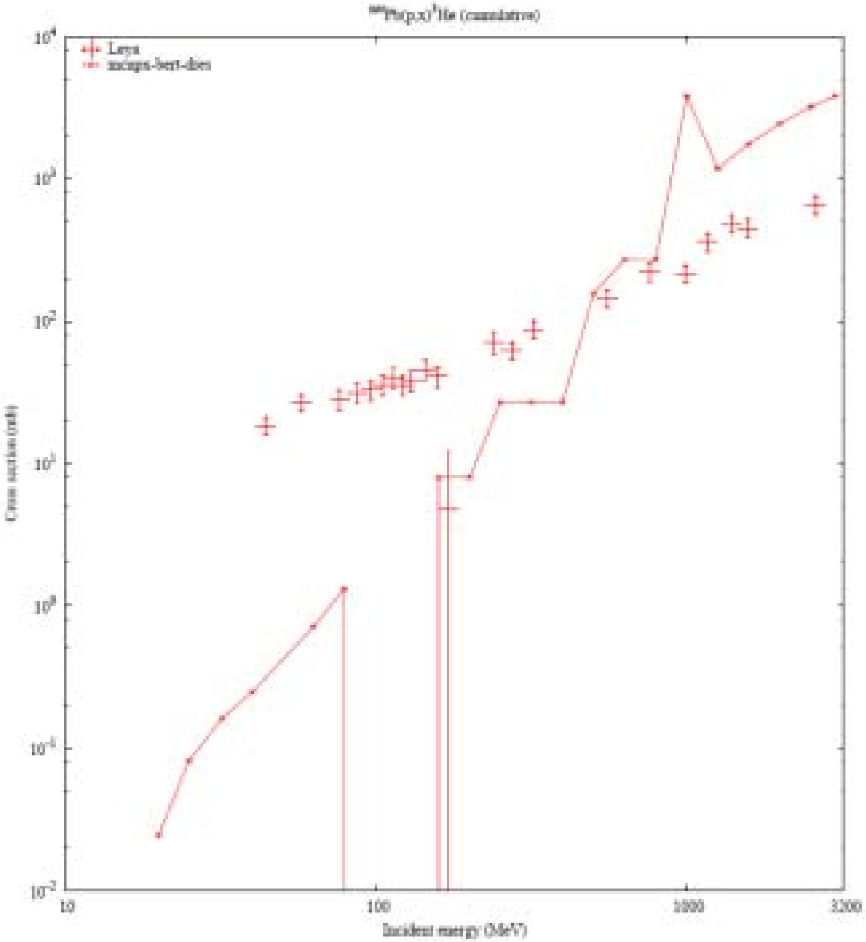
Excitation Functions Fe-nat (cont.)

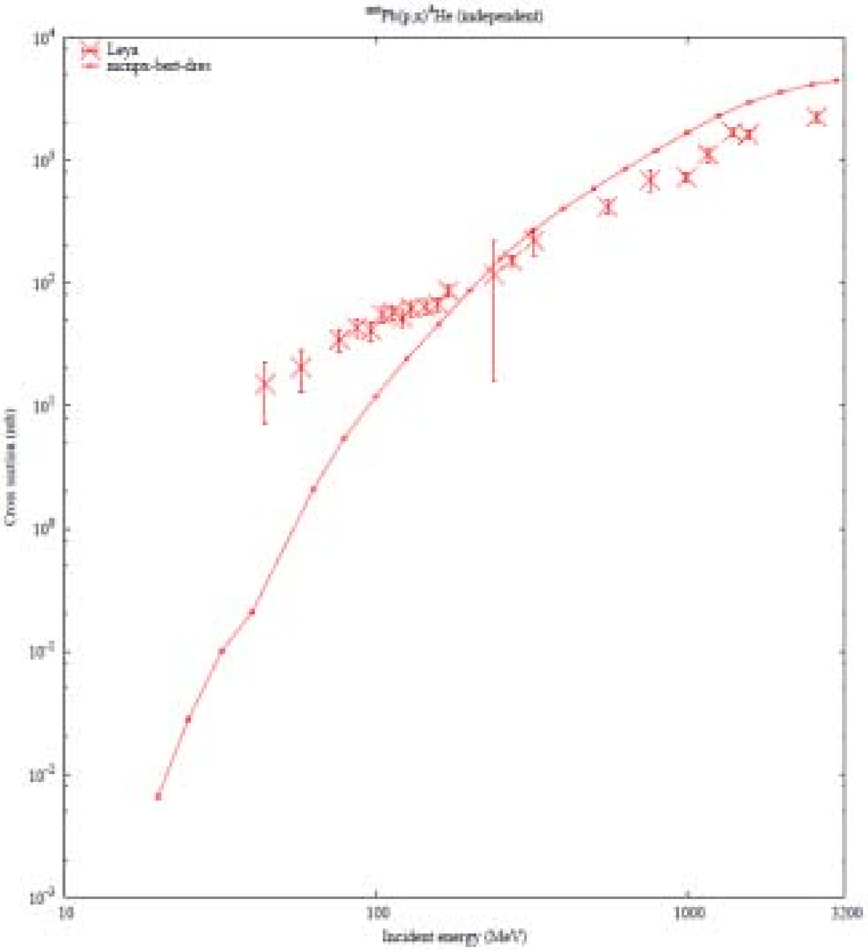




- **Target-near residuals are ok**
- **Must look into gaps and dips (treatment of metastables in post-processing)**

Excitation Functions Pb-nat

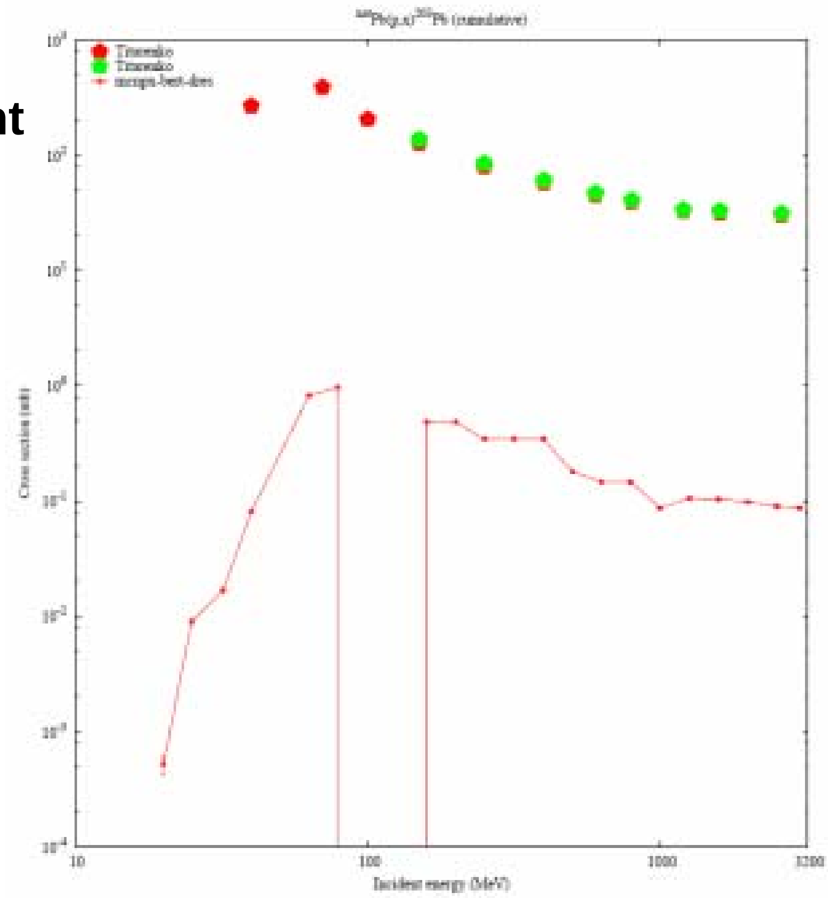




- **overpredict He production above 800 MeV, underpredict below**

Excitation Functions Pb-nat (cont.)

Again metastable treatment



- **82 203 2.2045e+01 1.9841e-02**
- **182 203 7.2210e+00 1.0832e-02**
- **282 203 1.6603e-01 1.6769e-03**

Outlook

- Bertini-Dresner needs a lot of improvement
- Bertini is at stage of 1973, needs better integration to preequilibrium
- Dresner saw some attention but not in MCNPX -> HERMES ->GEM
- Fission models are at stage from 1980 -> new Atchison model?

ORNL is not working on Bertini and Dresner for many years