The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

**1930-19**

# Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions

***4 - 8 February 2008***

## Summary and perpectives (intercomparison description)

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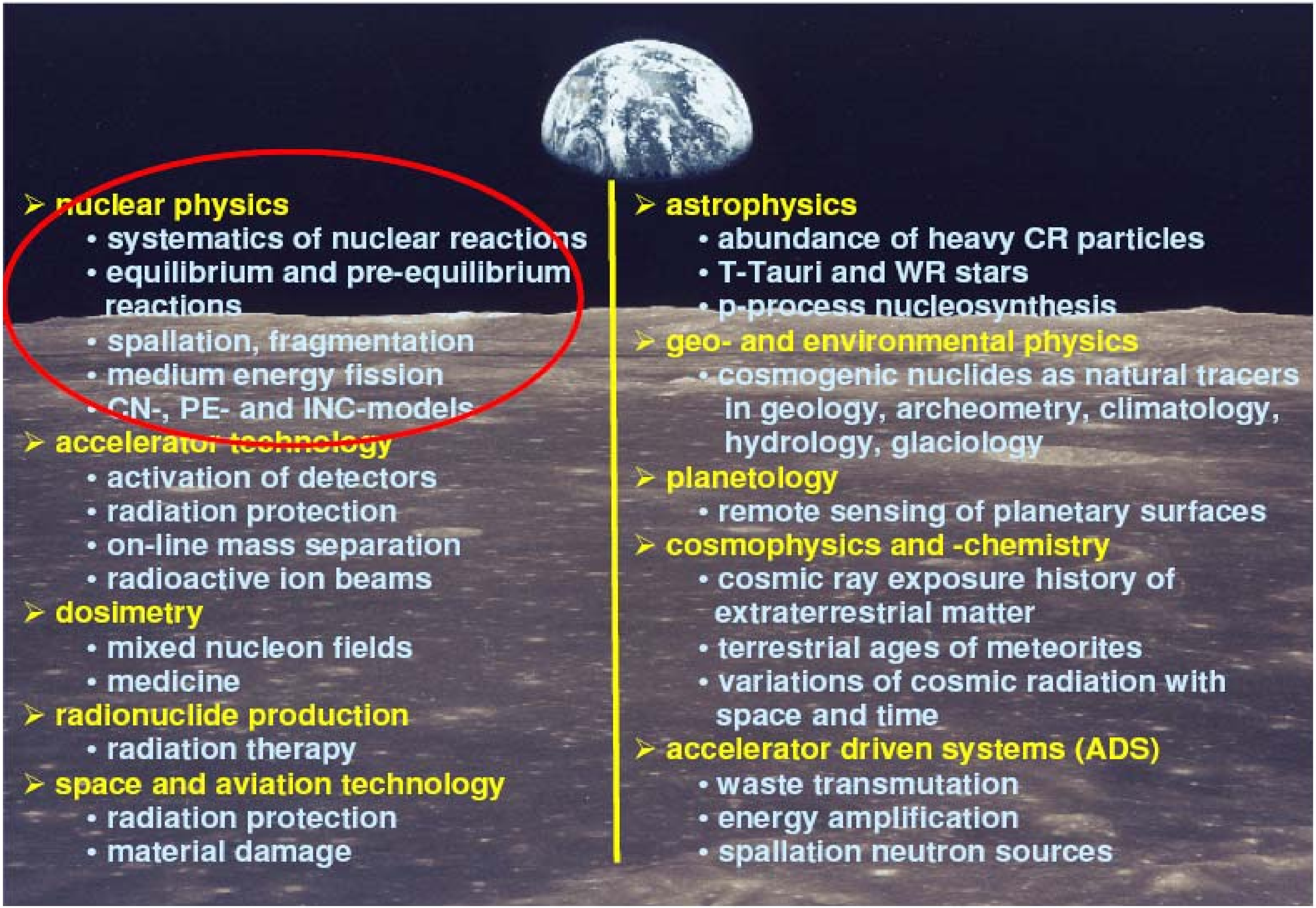
# Summary and perspectives

Sylvie LERAY

CEA/Saclay, DAPNIA/SPhN


➢ nuclear physics
• systematics of nuclear reactions
• equilibrium and pre-equilibrium reactions
• spallation, fragmentation
• medium energy fission
• CN-, PE- and INC-models
➢ accelerator technology
• activation of detectors
• radiation protection
• on-line mass separation
• radioactive ion beams
➢ dosimetry
• mixed nucleon fields
• medicine
➢ radionuclide production
• radiation therapy
➢ space and aviation technology
• radiation protection
• material damage
➢ astrophysics
• abundance of heavy CR particles
• T-Tauri and WR stars
• p-process nucleosynthesis
➢ geo- and environmental physics
• cosmogenic nuclides as natural tracers in geology, archeometry, climatology, hydrology, glaciology
➢ planetology
• remote sensing of planetary surfaces
➢ cosmophysics and -chemistry
• cosmic ray exposure history of extraterrestrial matter
• terrestrial ages of meteorites
• variations of cosmic radiation with space and time
➢ accelerator driven systems (ADS)
• waste transmutation
• energy amplification
• spallation neutron sources

# Data required for the design of spallation sources

- **Neutron production**
  - number ➔ source efficiency
  - energy, spatial distribution ➔ target optimisation, damage in window and structures
  - high energy neutrons ➔ shielding
- **Charged particle production**
  - gas ($H_2$, He) production ➔ embrittlement, swelling
  - energy ➔ DPA, energy deposition
- **Residual nuclide production**
  - element distribution ➔ corrosion, change in metallurgical properties
  - isotope distribution ➔ activity (short lived isotopes), radiotoxicity (long lived isotopes), decay heat, delayed neutrons
  - recoil energies ➔ DPA in window and structures, energy deposition

## The importance of spallation reactions
## -------- in general --------

**Computer simulation** opens up new potentials to study physical and technical issues.

**Computer simulation** is sometimes the only way to understand  the complexity of physical phenomena.

The classical categories – theory and experiment – nowadays are completed by a third category – **THE COMPUTER SIMULATION.**

**BUT not to misunderstood:**

Computer simulation cannot  substitute experiments. It extends the field of science and enables experiments in a hypothetical world.

**The simulation models used, must be validated against experiments to demonstate their realibility, accuracy, and their predictive power.**

# Aim of the Workshop

**Demonstration and discussion of the state-of-the-art INCE /QMD event generators**

**- Model dependent and critical parameters, validity and deficiency etc.**

**- What model could be named as standard model in the energy range between 0.1 up to 3.0 GeV ?**

**Is it a dream to have only one model ??**

**Presentations of recent thin target experiments**

- **Double differential cross sections, reaction rates, multiplicities, excitation functions, residuals etc.**
- **Availability of the experimental data, corrections, accuracy etc.**

# Aim of the Workshop

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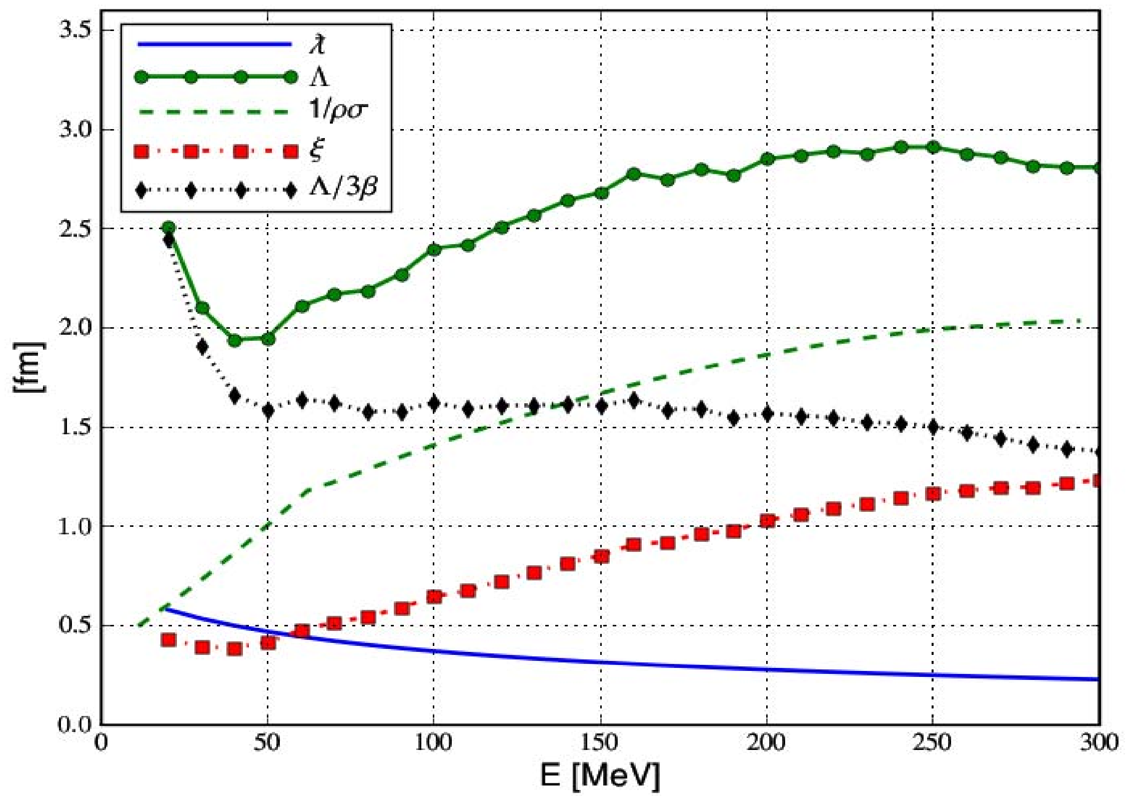
**Discussion, definition /or establish a <u>BENCHMARK</u> on spallation reactions of ‚thin' targets**

- **Defining the experimental data, which data should be used ?**
- **Which experiments ?**
- **Making a selection !!**
- **What is the best format to distribute the data ?**
- **Who should be responsible on collecting the data and will retrieve/disseminate them?**
- **Figures of merrit**
- **How much time is needed to finish and to present the <u>BENCHMARK</u> at a follow-up workshop?**
- **Who will participate ??**

# Intranuclear cascade models

# Central collision p+$^{208}$Pb




$$\lambda\!\!\!^{-} << d < \Lambda < R$$

$$\Lambda / 3\beta >\approx 1\, fm$$

$$\xi \equiv \Lambda / \lambda\!\!\!^{-} / 10$$

$$\xi > 1.0 \Rightarrow E >\approx 200.MeV$$

# Expected limitations

- $E_{inc}$> ≈ 50 MeV for:
  - Total nucleon yields
  - Peripheral collisions, e.g. “quasi-elastic”,(p,2p)
- $E_{inc}$ > ≈ 200 MeV for:
  - “Violent reactions” (high multiplicity, high excitation energy)

**Significant discrepancies expected for outgoing particles for $E_{inc}$ lower than few tens MeV**

**and for very light targets**

# Model presentations

- **Intra-nuclear cascade**
  - ISABEL and future ETGAR (Y. Yariv)
  - INCL4 (A. Boudard)
  - CEM and LAQGSM (S. Mashnik)
  - PEANUT (FLUKA) (A. Ferrari)
  - JAM (K. Niita)
- **QMD, VUU, BUU**
  - BUU (Z. Rudy)
  - IQMD (C. Hartnack)
  - JQMD (K. Niita)
- **De-excitation models**
  - SMM (A. Botvina)
  - GEMINI (R. Charity)
  - ABLA (K.H. Schmidt)
  - GEM (S. Mashnik)

# Deliberate choice of authors:

- A model with physical (justified?) ingredients
- Reduced phenomenology (or fitting processes)

| |
|---|
| For a better understanding of the reaction mechanism |
| ... and the hope to be more predictive in extrapolations |

- Even if possibly less precise as event generator

# Event generators for applications must:

- Be universal and describe arbitrary reactions without any free parameters
- Provide as good as possible agreement with available experimental data and have a good predictive power
- Not require too much computing time

# Formation zone* *(→ classical INC will never work)*

Naively: "materialization" time (J.Ranft, L.Stodolski).
Qualitative estimate:

In the frame where $p_{//}=0$

$$\bar{t} = \Delta t \approx \frac{\hbar}{E_T} = \frac{\hbar}{\sqrt{p_T^2 + M^2}}$$

Particle proper time

$$\tau = \frac{M}{E_T}\bar{t} = \frac{\hbar M}{p_T^2 + M^2}$$

Going to the nucleus system

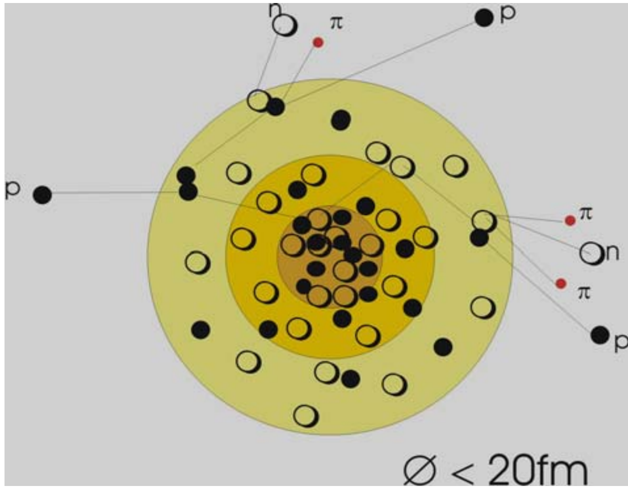
$$\Delta x_{for} \equiv \beta c \cdot t_{lab} \approx \frac{p_{lab}}{E_T}\bar{t} \approx \frac{p_{lab}}{M}\tau = k_{for}\frac{\hbar p_{lab}}{p_T^2 + M^2}$$

Condition for possible reinteraction inside a nucleus:

$$\Delta x_{for} \leq R_A \approx r_0 A^{\frac{1}{3}}$$

* J.Ranft applied the concept, originally proposed by Stodolski, to hA and AA nuclear interactions

# *Boltzmann-Uehling-Uhlenbeck (BUU) model:*

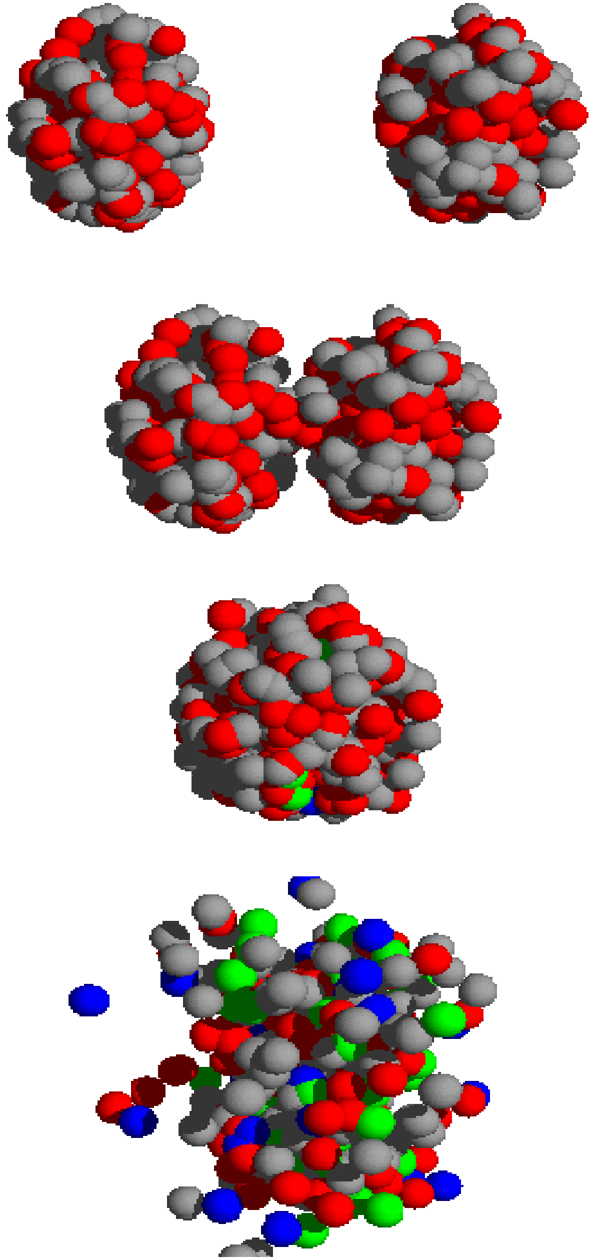



- ***Classical Boltzmann transport equation with Pauli blocking factors***
- ***p + A collision is described as cascade of N + N collisions***
- ***between collisions nucleons are moving mean field being a function of nuclear density inside nucleus***
- ***the equation is solved using Monte Carlo method, generating positions and momentum of particles in successive time steps***

***K. Niita, W. Cassing and U. Mosel, Nucl. Phys. A 504(1989)391***
***G. F. Bertsch and S. Das Gupta, Phys. Rep. 160(1988)189***

# What is IQMD?

**Not MCNP!**



- **semiclassical model with quantum features**

- **microscopic N-body description**

- **calculation of heavy ion collisions on an event-by-event-basis**

- **includes N, Δ, π with isospin d.o.f.**

- **potentials of Skyrme type for describing nuclear eos**

# Conclusions:

- *Two – stage scenario of the proton induced spallation reactions (combined **BUU + GEM** model ) gives good description of neutron and proton spectra*
- *In case of other ejectiles H, He, Li, ... – only low energy part of spectrum is described – high energy part description needs implementation of coalescence processes into the first stage models*
- *Proton induced spallation as rather non-invasive process*
- *Properties of residual nuclei depend weakly on proton impact energy, strongly on target mass*

# Conclusion?

**Rather a discussion  than a conclusion...**

**IQMD is working well for A+A but not well tested for p+A.**

**Problems when describing fragmentation, particle production and collectif effects (flow) at the same time.**

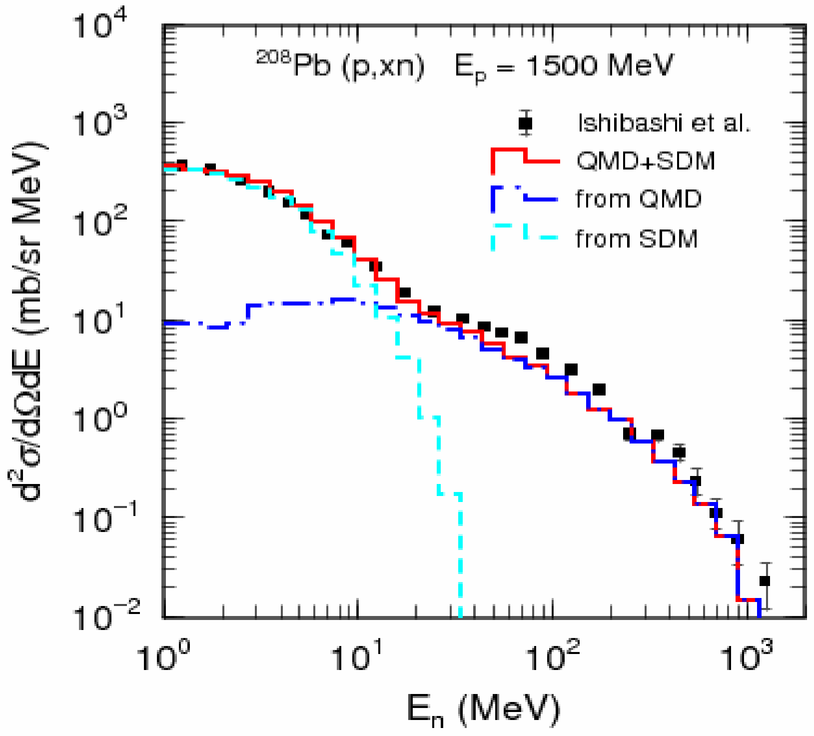
**There are several parameters which might be used for finetuning, but the observables have to be discussed.**

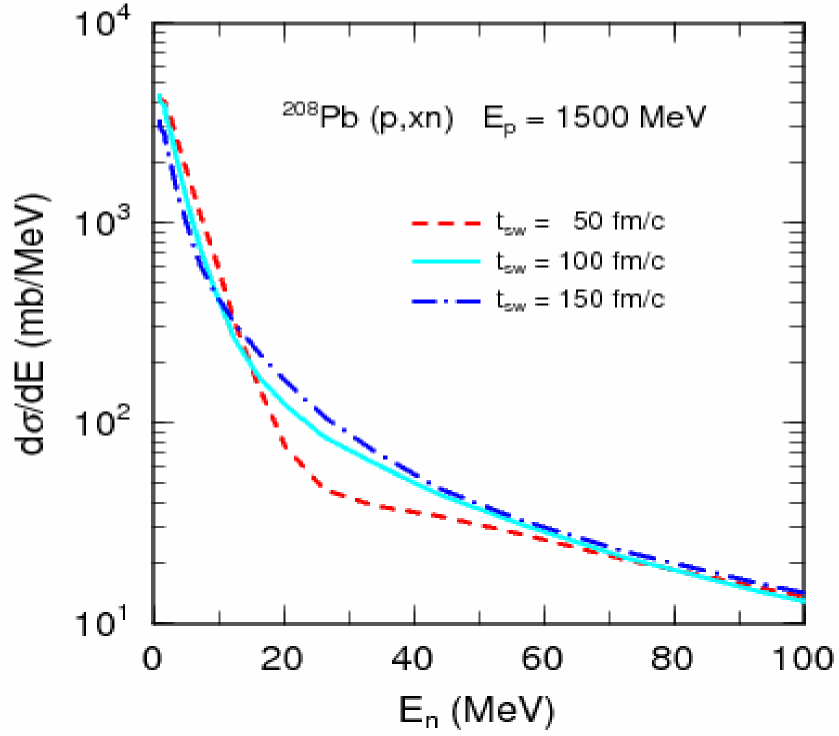
**Maximum energy of application is around 2-3 GeV:**

**Above, use UrQMD**

# QMD + SDM (Statistical Decay Model)

At the end of the dynamical stage, the QMD simulation yields many nucleons and fragments which are normally in highly excited states. We stop the QMD calculation and switch to the statistical decay model (SDM) at the end of the dynamical stage.
The final results are not sensitive to the switching time if we use the switching time from 100 fm/c to 150 fm/c.



## Limitations and Problems in JAM

- Fixed target potential :
  no dynamical change of nucleus,
  no cluster emission in the dynamical stage

## Limitations and Problems in JQMD

- Nucleus : described as a self-binding system
  dynamical change of nucleus,
  cluster emission ??

- ground state is not a energy minimum state
  → spontaneous emission of nucleons
- not fully relativistically covariant
  → unstability of nucleus after boosting

} Solved by new R-JQMD (Relativistic JQMD) by D. Mancusi

- connection time to statistical model
  → over cooling of the residual nucleus

# De-excitation models

## Conclusions on nuclear multifragmentation:

Multifragmentation of nuclei is fast decay process taking place in all reactions where high excitation energy is reached. It dominates over sequential evaporation and fission which are usual at low energy.

Multifragmentation takes as much as 10-15% of the total cross section in high energy hadron nucleus reactions, and much more for high energy nucleus-nucleus collisions. It must be included in hybrid calculations of particle transport in complex matter: nuclear transmutation (environment studies), electro-nuclear breeding (new methods of energy production), proton and ion therapy (medical research), radiation protection of space detectors (space research). Multifragmentation can be the dominating channel for production of some particular isotopes.

Multifragmentation can be interpreted as a manifestation of the liquid-gas type phase transition in finite nuclei, and it allows for investigating the phase diagram of nuclear matter. In particular, one can investigate properties of hot nuclei/fragments surrounded by other nuclear species.

# Conclusions

- GEMINI has the correct treatment of angular momentum
- GEMINI seems to work reasonable well for light compound nuclei, but I am not sure why.
- GEMINI doesn't work for heavy systems-problems with the fission yield and width of mass distribution

  a) few dimensions

  b) new barriers will help (Wigner Correction?)

  c) Could interpolate from systematic of fission mass distributions

  after including fission delays and saddle-to-scission time.

  d) A simplistic scission-point model for mass distributions gives good results (could include shell effects to get double humped distributions)
- Lower Coulomb barriers for alpha + Li+Be. emission for heavy systems
- Large temperature dependence of level-density parameter for heavy systems

# ABLA07

Developed by

A. Kelic, M.V. Ricciardi, K.-H. Schmidt

New features (with moderate increase of computing time):

- Multifragmentation
- CN-decay channels γ, n, p, LCP, IMF, fission (continuous)
  - inverse x-sections from nuclear potential
  - treatment of angular momentum
  - fission transients from Fokker-Planck equation
  - barrier structure in low-energy fission
  - nuclide production in fission with 1 parameter set
    - from spontaneous fission to high E* for all CN
  - evaporation on fission path

Ready to be coupled with INCL 4 (or other INC, or ABRA, or ..)

# Intercomparison specifications

# Specifications

- **Domain: N + A, 20 MeV to 3 GeV, A >11**

**why 20 MeV?**

- ➥ **20-150 MeV libraries not available for all isotopes**
- ➥ **for residue production below 150 MeV**
- ➥ **to calculate correlations between particles**

# *Event Generator Mode for low energy neutrons in PHITS*

Neutron data + Special Evaporation Model

We use the channel cross sections and neutron energy spectrum of the first neutron and assume the binary decay of recoiled nucleus.

**Neutron channels**

| Channel | | |
|---|---|---|
| **capture** | $\Gamma_n = 0$ | charged particle and photon decay |
| **elastic** | | final state is uniquely determined |
| **(n,n')** | $\Gamma_n = 0$ | charged particle and photon decay after the first neutron emission |
| **(n,Nn')** | $\Gamma_n \neq 0$ | all particle and photon decay after the first neutron emission |

By this model, we can determine all ejectiles (neutrons, charged particles, nucleus and photons) with keeping energy and momentum conservation.

PHITS can transport all charged particle and nucleus down to zero energy and estimate deposit energy without local approximation (kerma factor).

# Specifications of the intercomparison

- Participants should be able to treat the complete reaction mechanism
  - ➥ complete reaction description (INC/QMD + De-ex)
- Participants should calculate the whole mandatory set of experimental data
  - ➥ + additional set if they have enough time
- Participants should give a comprehensive description of ingredients and parameters
  - ➥ list of the main ingredients and parameters
  - ➥ additional information requested ($E^*$, $A_R$, …)
- Calculations with one model should be done with the same set (default) parameters
  - ➥ predictive power

# List of the main ingredients and parameters

- **INC, INC+PE, QMD, BUU**
  - NN interaction elastic and inelastic
  - in medium corrections
  - Nuclear potential : $V_N$,$V_\pi$
  - Nuclear shape
  - Coalescence: parameters
  - Pre-equilibrium
  - Stopping criterium
  - Computational time
  - Range of validity
  - …

- **Dexcitation models**
  - level densities
  - $\sigma_{inv}$
  - fission barriers
  - fission fragment distributions
  - …

# Additional information on the calculation

- model $\sigma_R$ ($\sigma_{geom}$x$N_{inel}$/$N_{evts}$)
- $\sigma'_R$ used (normalisation)
- E*, E*/$A_R$, $A_R$, $Z_R$, $P_R$, $J_R$ distributions to enter de-excitation, bidim E*-$A_R$, ntuple
- Multiplicities of n, p, π, lcp, IMFs from 1st stage and de-excitation, ntuple

# Choice of experimental data

- neutron: DDXS, multiplicity distributions, average multiplicities
- p, light charged particles : DDXS, multiplicity distributions, average multiplicities
- π : DDXS, multiplicity distributions, average multiplicities
- residues (including IMFs): isotopic distributions, excitation functions, recoil velocities
- Coincidence measurements
- Not (yet) existing data

# Choice of experimental data

# Proposed set of neutron data

- **Double differential cross-sections (p,xn)**
  - **Stamer data : Al, Zr, Pb at 256** MeV**
  - **Saturne data: Fe, Pb at 800, 1200, 1600 MeV, Al, Zr, Th at 1200 MeV**
  - **KEK data: Fe, In, Pb at 3 GeV**
  - **Lower energy data: 100 MeV (not 113) ??, Louvain 63 MeV??**
- **Multiplicity distributions**
  - **NESSI data: Al, Fe, Zr, Pb, U at 1.2 GeV**
- **Average multiplicity above and below 20 MeV**
  - **Saturne data: Fe, Pb at 800, 1200, 1600 MeV**

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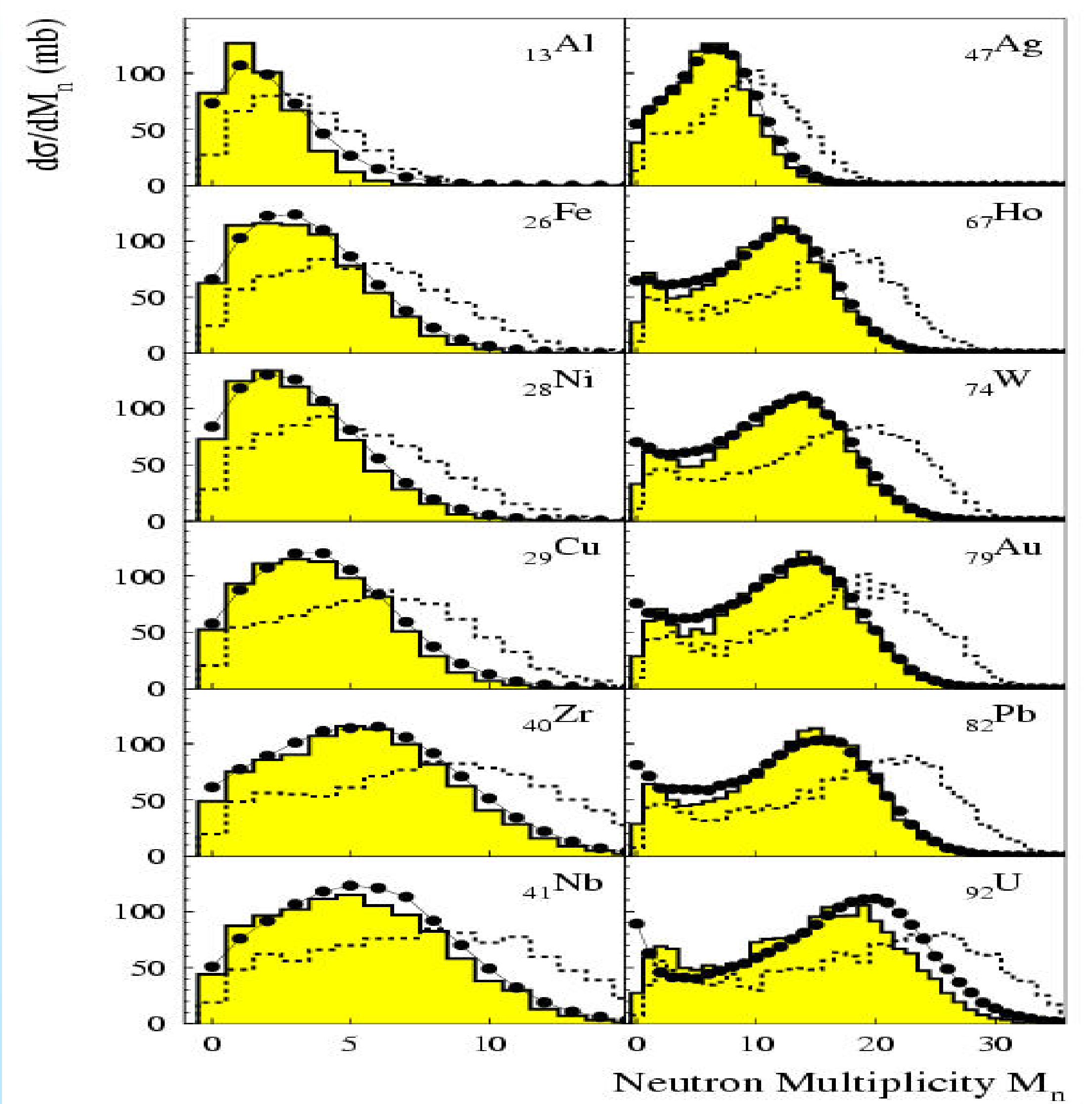
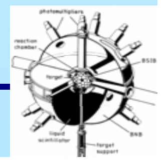
# Neutron multiplicity distributions for 1.2 GeV p+Al,...,U.




measured (symbols) and calculated (histograms) neutron multiplicity distributions.

calculated (INCL2.0+GEMINI) distributions are shown before (dashed histogram) and after (shaded histogram) folding with the neutron energy dependent detector efficiency.

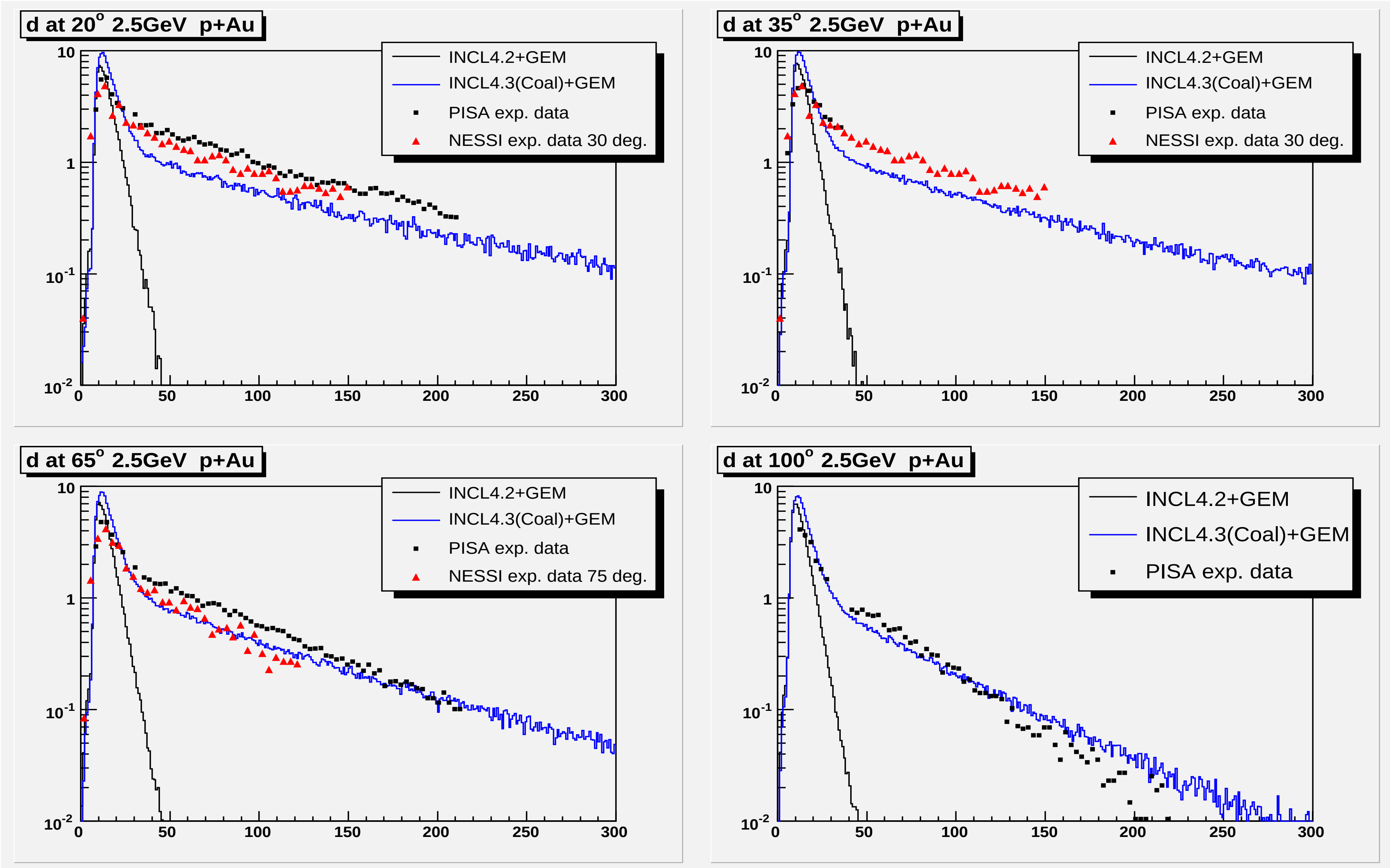
note different $M_n$ scales for the left and the right panels.



# Proposed set of LCP data

- **Proton double differential cross-sections (p,xn)**
  - LANL (p,xp) 800 MeV, Pb (and Fe?)
  - (p,xp), 500 MeV p+Ni, Ta
  - p, LCP 160 MeV A. Cowley, PR C54 (1996) 778
  - p, LCP, n+Cu, Bi 542 MeV
  - p, LCP, NESSI/PISA data: p+Au 1.2 and 2.5 GeV
  - PISA data: p+Ni 175 MeV
  - Bertand-Pelle, PRC 8 (1973), 63 MeV
- **Production XS**
  - $^{3}He$, $^{4}He$ on Fe and Pb excitation function from threshold to 2.6 GeV R. Michel + Y. Titarenko + NESSI
  - d, t

# Comp.NESSI/PISA -INCL4.X 2.5 GeV p+Au



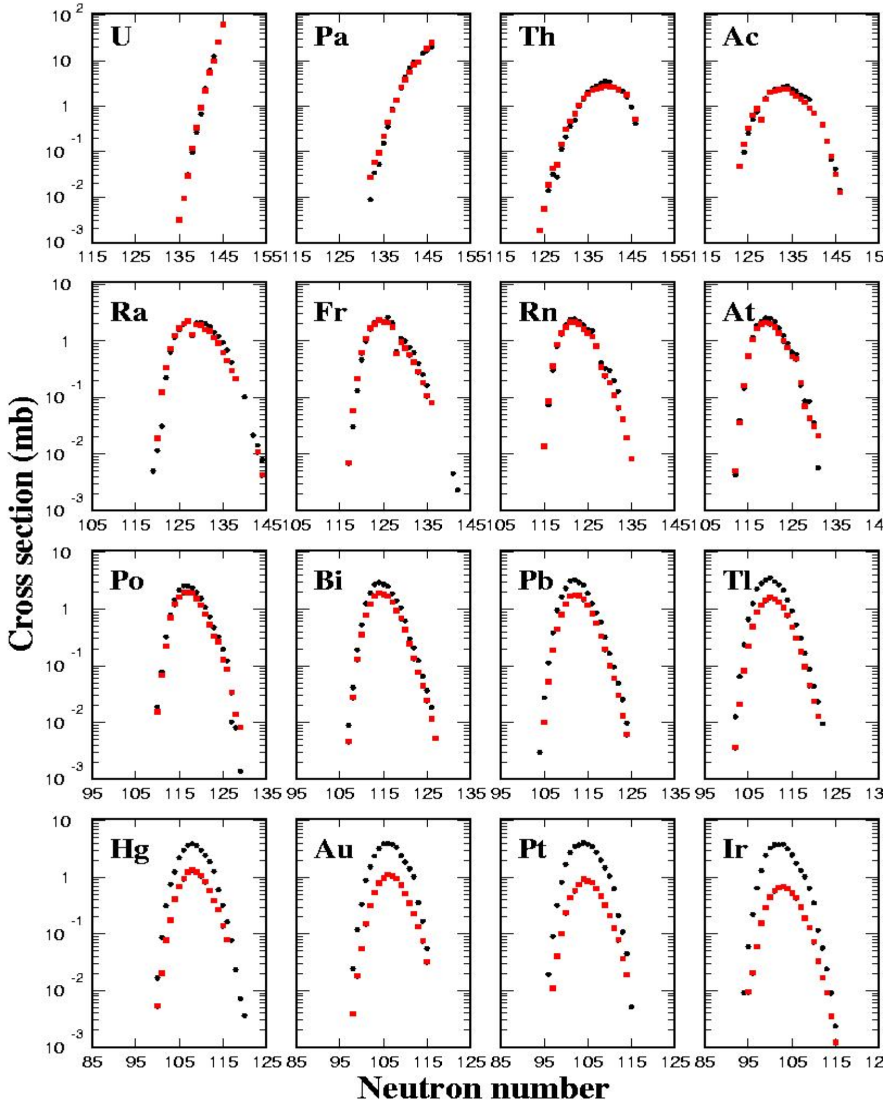
# Proposed set of pion data

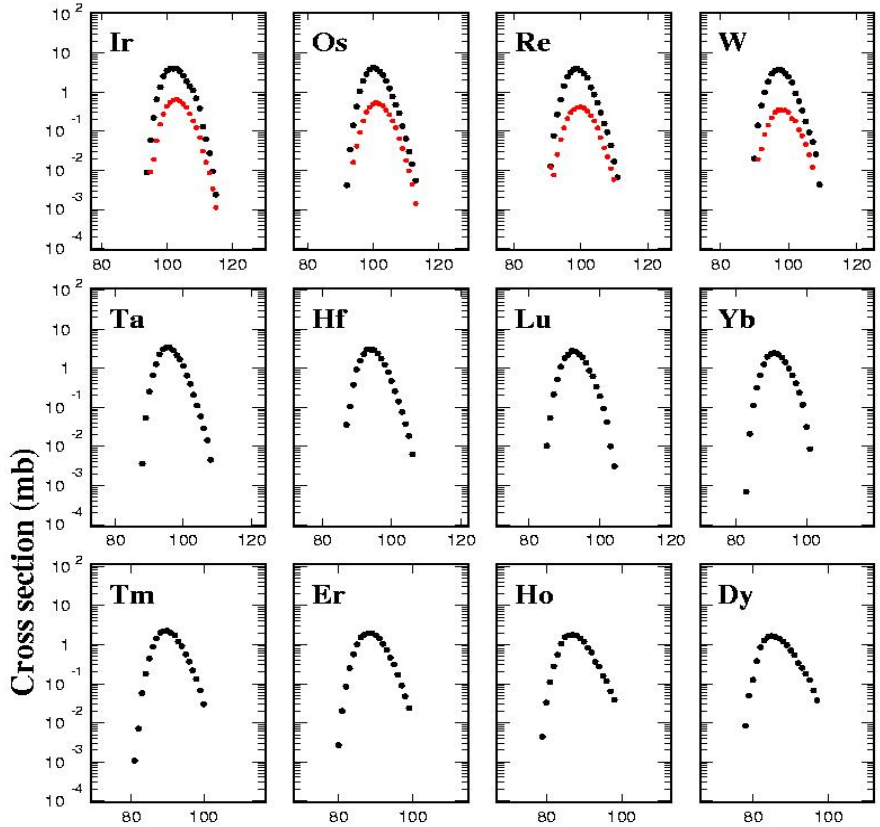
- **Pion double differential cross-sections (p,xπ)**
  - **Cochran data p, π+, π-, 743 MeV**
  - **PSI 590 MeV π+, π- several targets**
  - **3 GeV/c PL 159B, 1 (1995)**

# Proposed set of residue data

- Isotopic XS
  - Fe: 300, 500, 750, 1000, 1500 MeV
  - Xe: 200, 500, 1000 MeV
  - Pb: 500, 1000 MeV
  - U: 1000 MeV
- Excitation functions
  - Fe
  - Nb
  - Pb
  - U
- Other data
  - NESSI/PISA IMF DDXS Au, 1.2 GeV
  - Light system, p+C 1 GeV isotopic and excitation function
  - Coincidence data: NESSI LCP versus Mn, SPALADIN

# Results: Isotopic Production Cross Sections



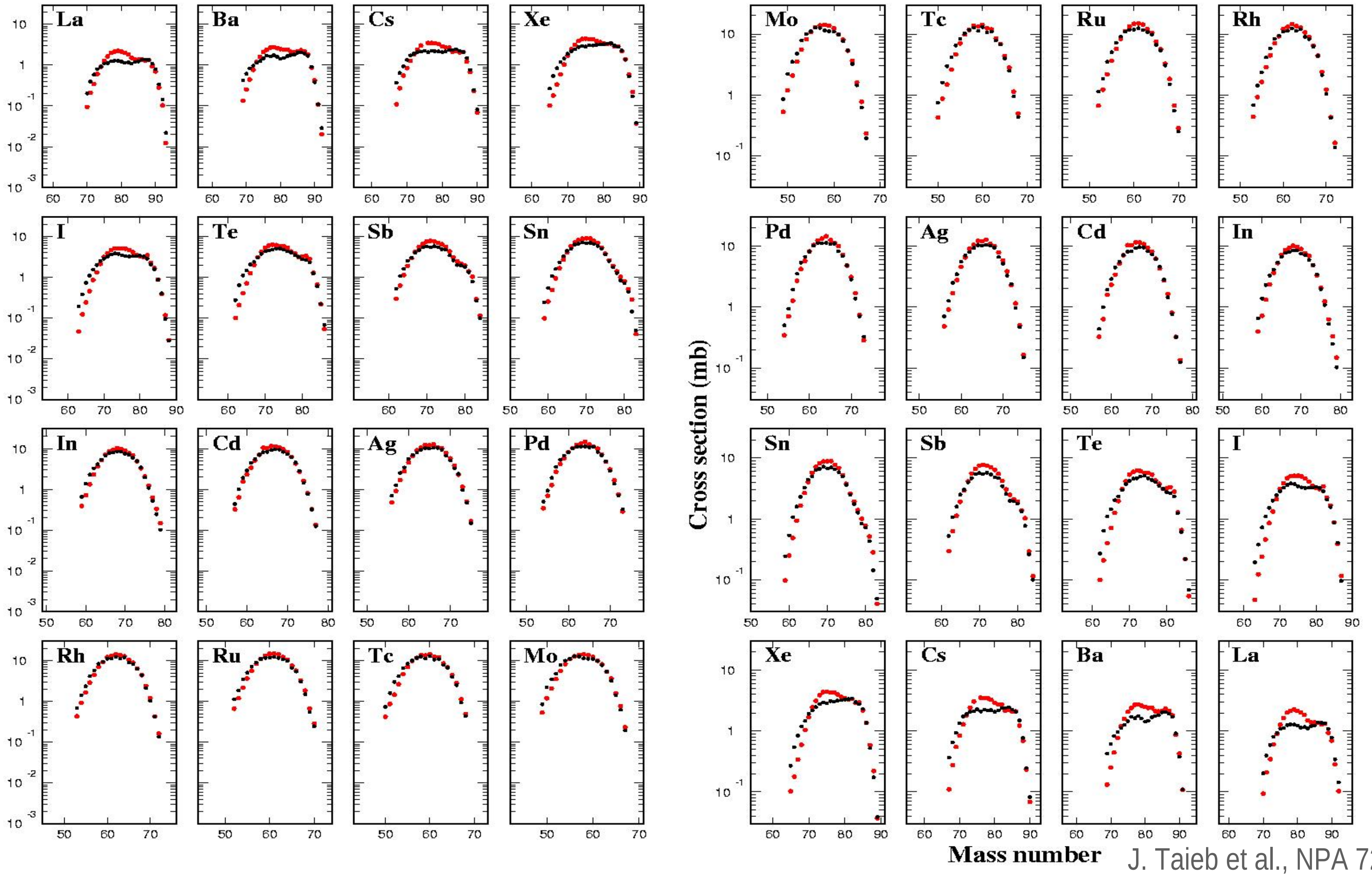

$^{238}$U(1 A GeV) + p

$^{238}$U(1 A GeV) + d

Evaporation residues

M. Bernas et al., NPA 725 (2003) 213
E. Casarejos et al., PRC 74 (2006) 044612

# Results: Isotopic Production Cross Sections




$^{238}$U(1 A GeV) + p

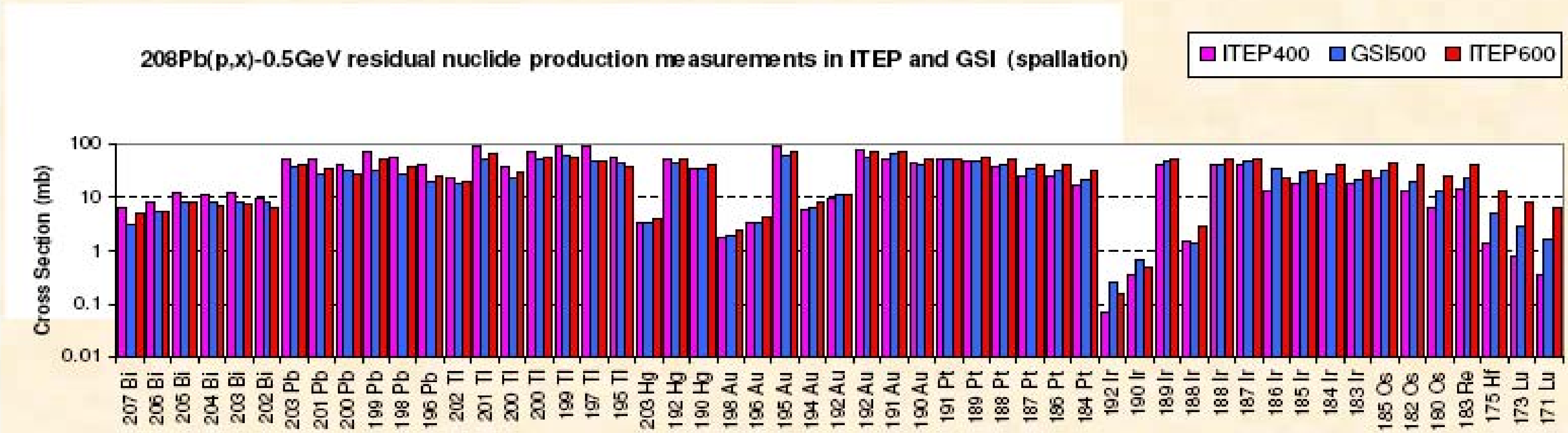
$^{238}$U(1 A GeV) + d

Fission residues

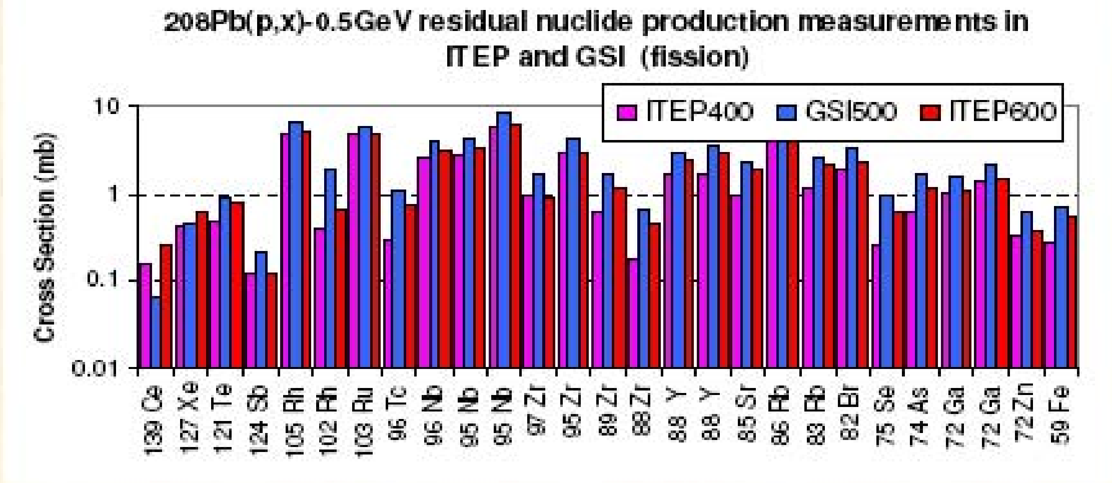
J. Taieb et al., NPA 724 (2003) 413

J. Pereira et al., PRC 75 (2007) 014602

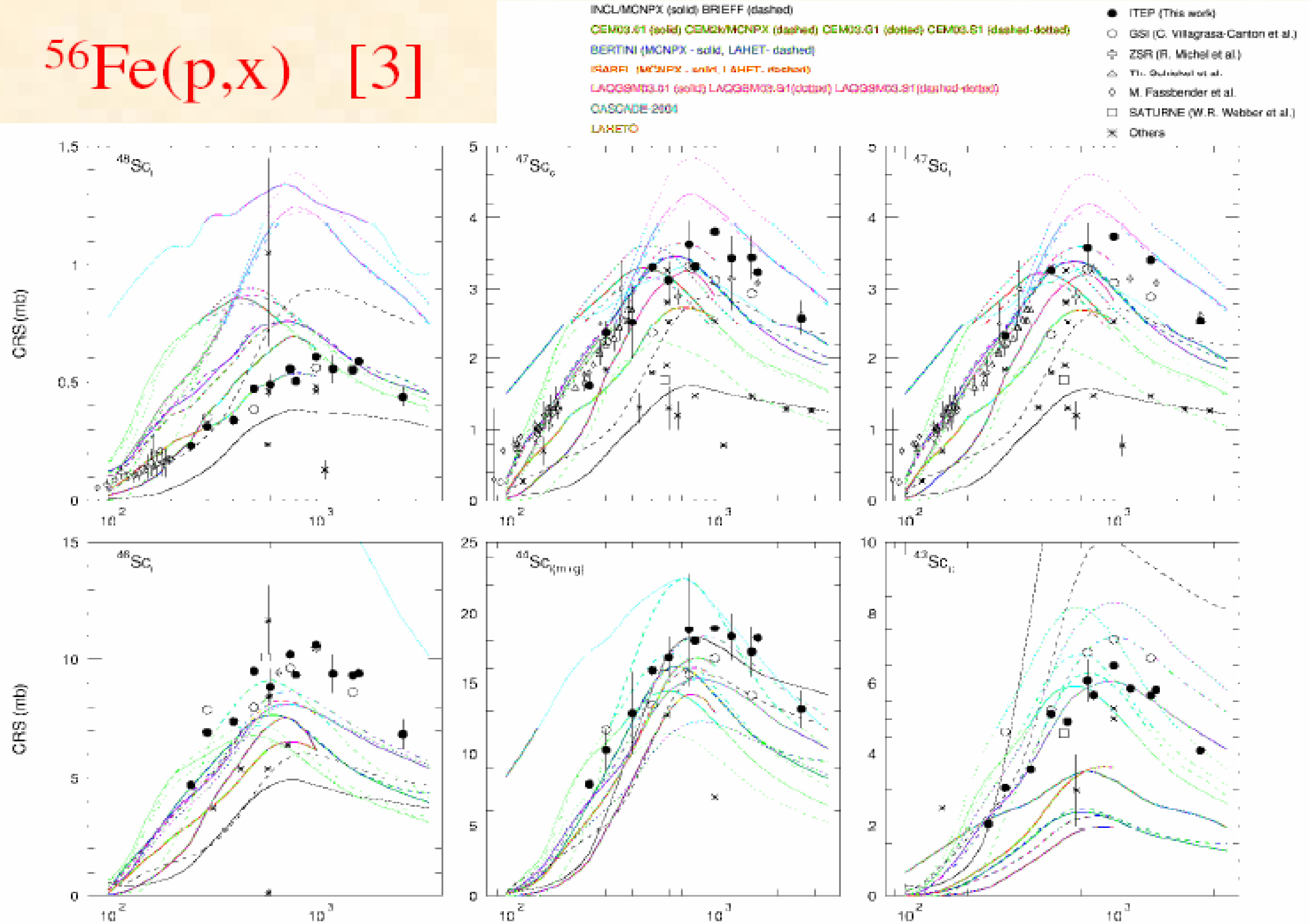
# $^{208}$Pb(p,x)-0.5GeV: ITEP, GSI

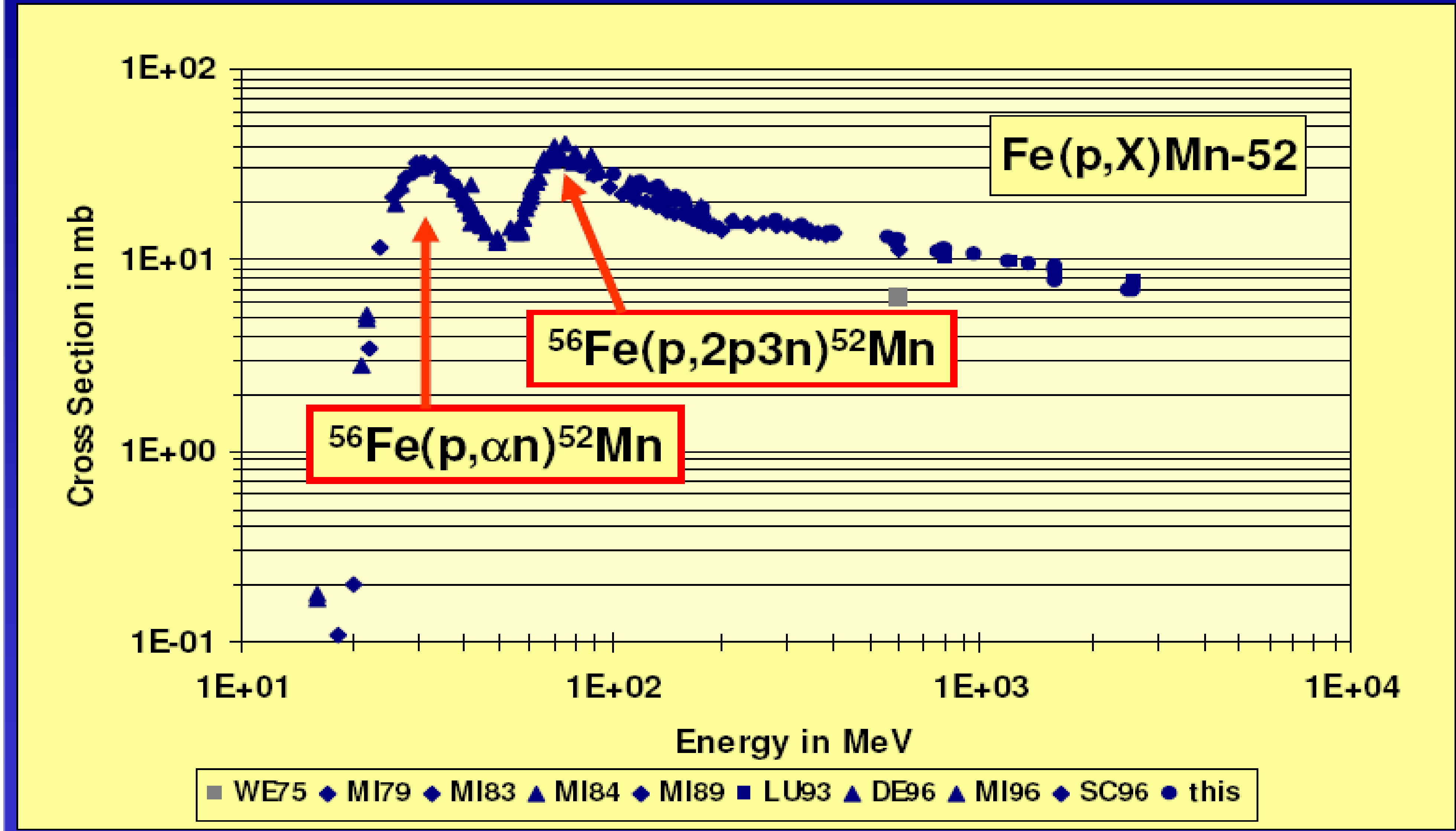



| | <F> | <ITEP/GSI> |
|---|---|---|
| All products | 1.51 | 0.98 |
| Spallation pr. | 1.32 | 1.12 |
| Fission pr. | 1.81 | 0.71 |



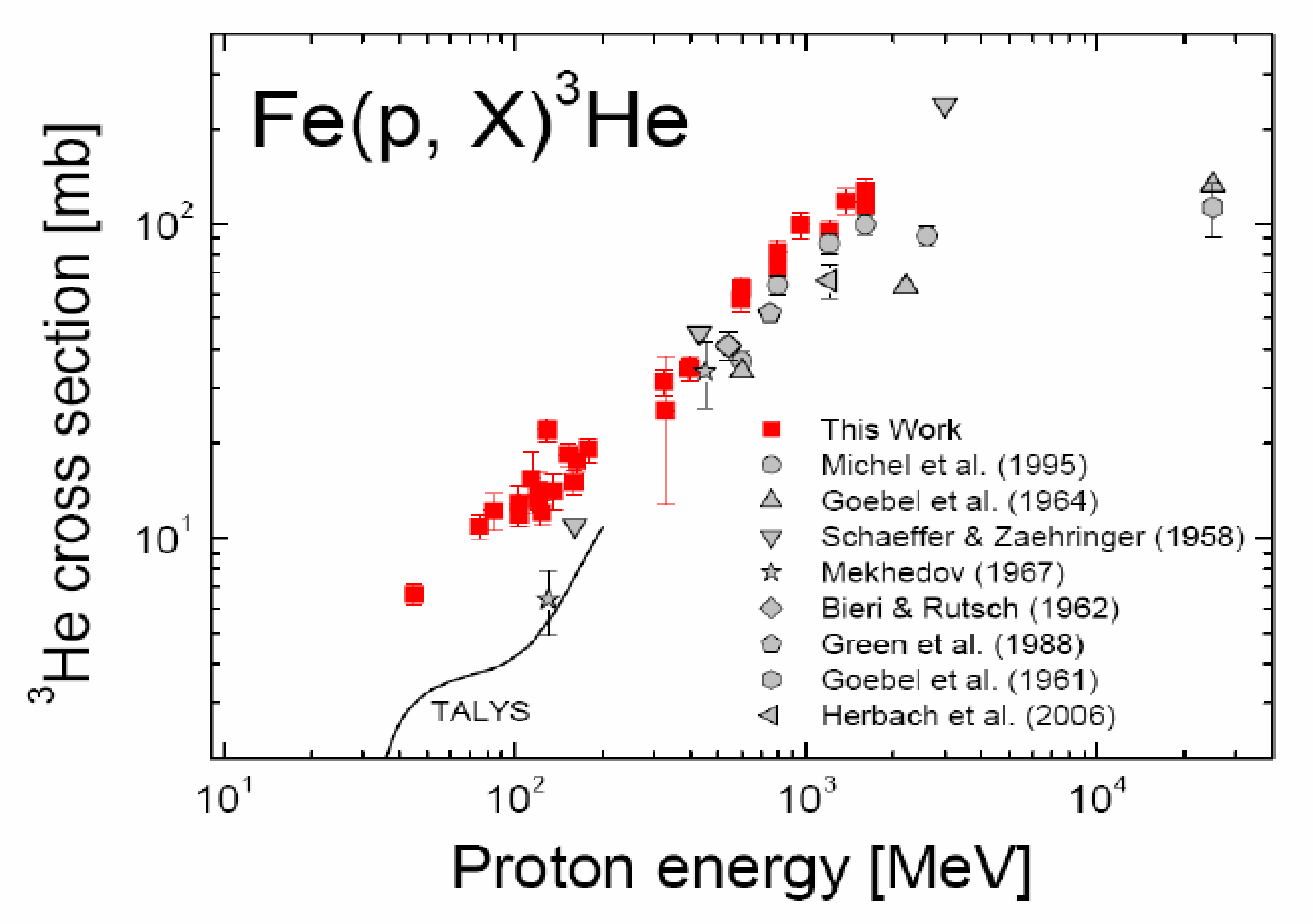
# $^{56}Fe(p,x)$   [3]


INCL/MCNPX (solid) BRIEFF (dashed)
CEM03.01 (solid) CEM2k/MCNPX (dashed) CEM03.G1 (dotted) CEM03.S1 (dashed-dotted)
BERTINI (MCNPX - solid, LAHET- dashed)
LAQGSM03.01 (solid) LAQGSM03.S1(dotted) LAQGSM03.S1(dashed-dotted)
CASCADE-2004
LAHET0
ITEP (This work)
GSI (C. Villagrasa-Canton et al.)
ZSR (R. Michel et al.)
M. Fassbender et al.
SATURNE (W.R. Webber et al.)
Others
CRS (mb)




R. Michel, ZSR, Leibniz Universität Hannover

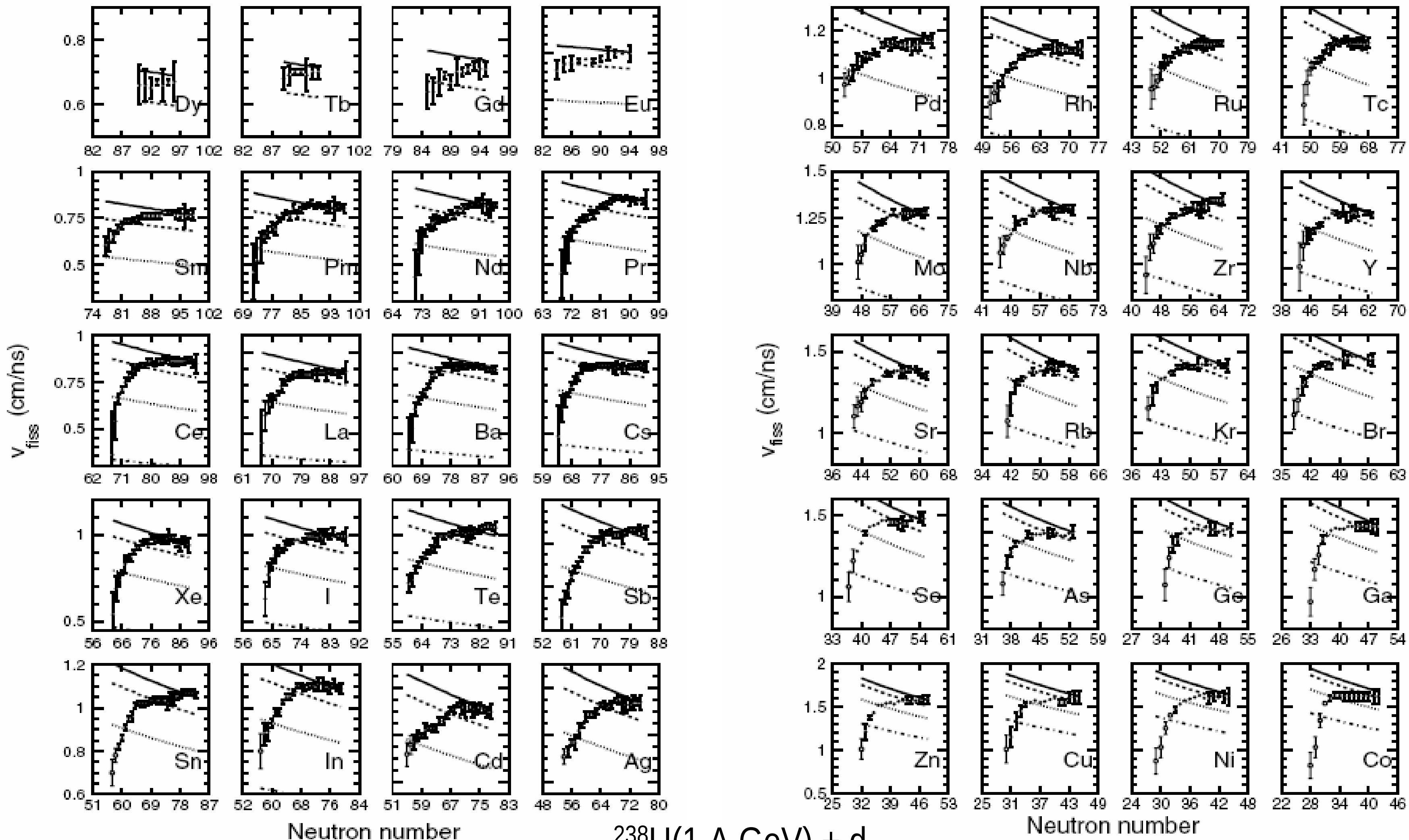
# Production of Helium




Ammon et al. (2008)

R. Michel, ZSR, Leibniz Universität Hannover

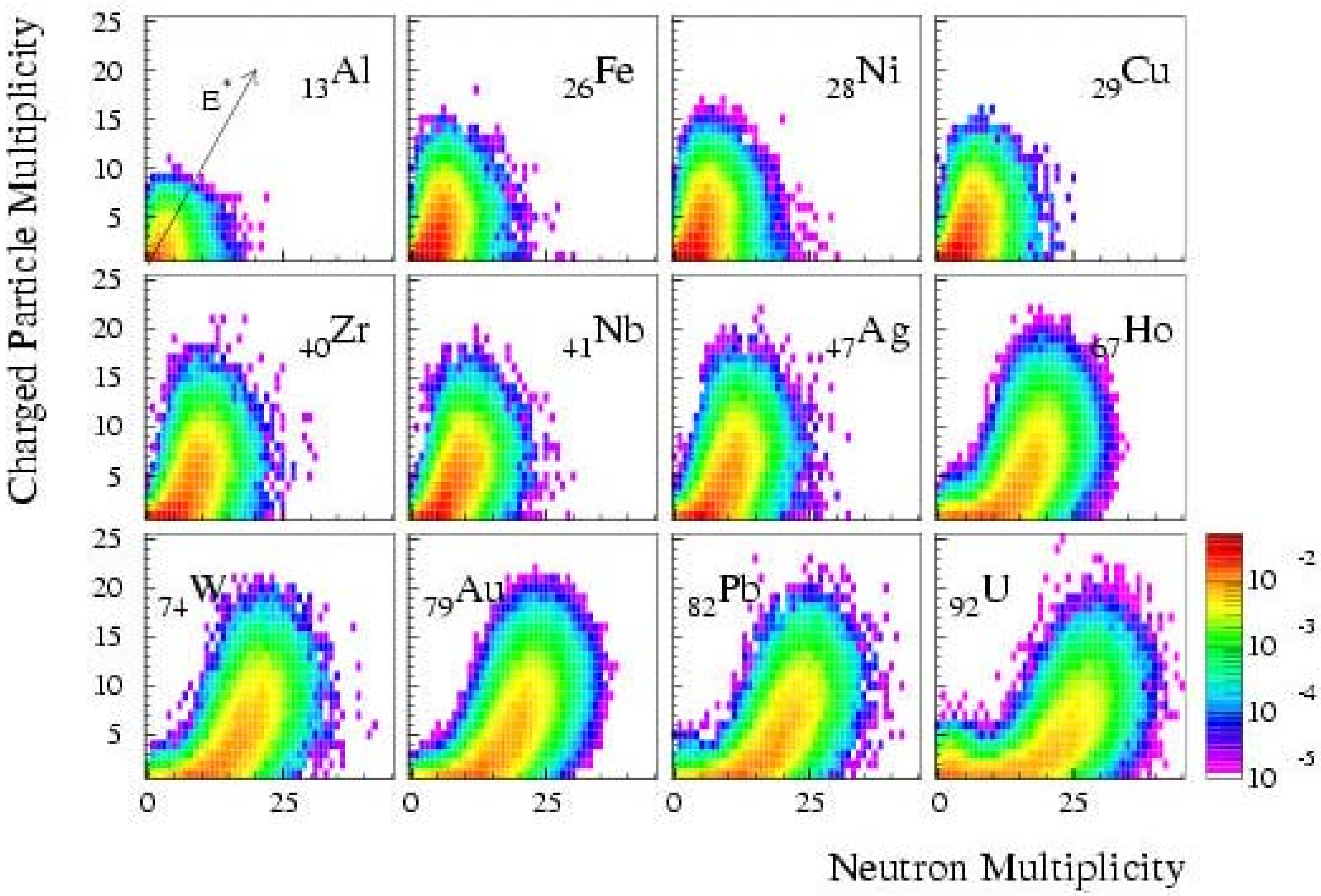
# Results: Velocity distributions




$^{238}$U(1 A GeV) + d

J. Pereira et al., PRC 75 (2007) 014602

# Light particle production in spallation reactions induced by protons of 0.8 to 2.5 GeV incident kinetic energy (NESSI)




Correlation of measured LCP-vs. N-multiplicity for 2.5 GeV proton-induced spallation reactions

The color scale gives the relative yield for each target per multiplicity bin

Thermal excitation is following indicated arrow

Cf. D. Hilscher presentation

- **Data sent to**

**Jean-christophe.david@cea.fr**

**Website at IAEA**

**A. Mengoni and G. Sterzenbach**

**Deadlines**

- **For specifications of benchmark: 31/03/08**
- **For papers: 30/04/08**
- **For calculation results: 20/12/08**

- **May 2009: first discussions on the results of the intercomparison at AccApp (satellite meeting if possible) in Vienna**