

# Benchmark of Spallation Models

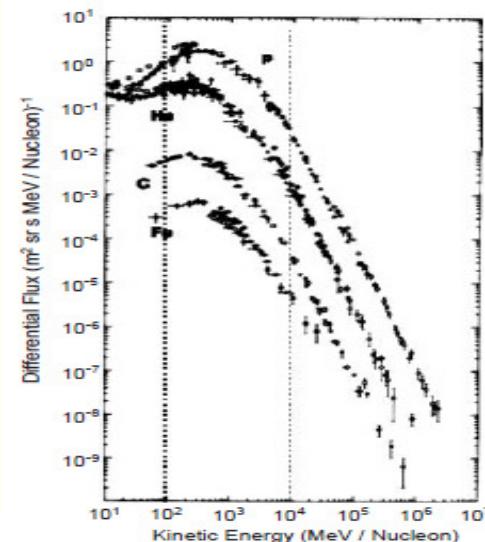
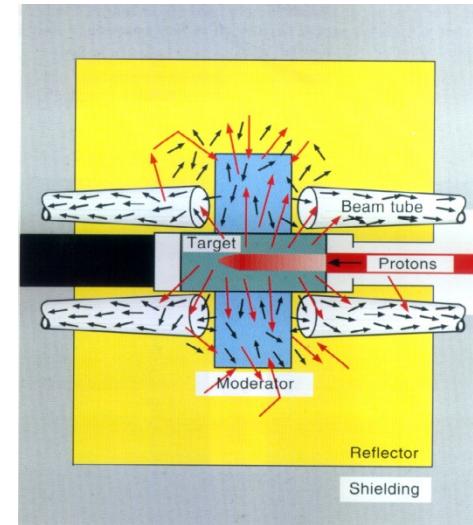
## Introduction

**Sylvie LERAY**

**CEA/Saclay, IRFU/SPhN**

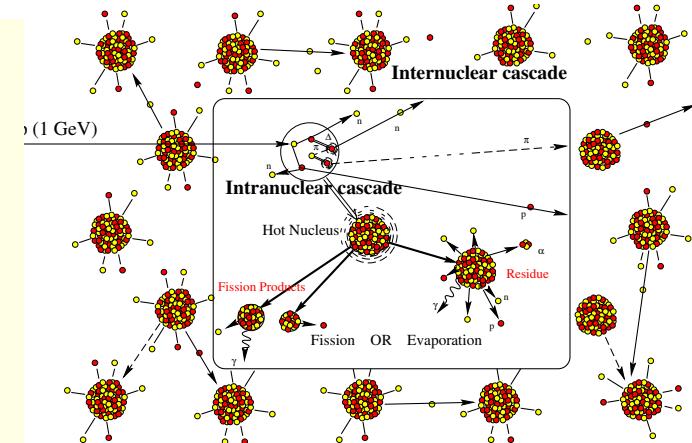
# Spallation reaction applications

- Spallation neutron sources
- ADS
- RIB production
- Detection setup simulation
- Radioprotection near accelerators
- Hadrontherapy
- Astrophysics
- Cosmic rays in space



# Simulation tools for spallation applications

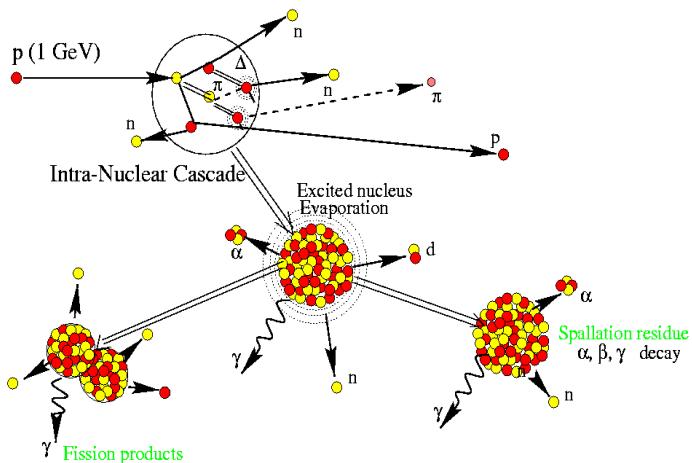
- Monte-Carlo transport codes  
→ propagation of all particles created in elementary interactions  
(MCNPX, FLUKA, GEANT4, PHITS...)



- Above 150-200 (20) MeV : nuclear physics models (Intra-Nuclear Cascade (+ Pre-eq) + evaporation-fission) → cross-sections, properties of emitted particles directly used by the transport codes
- Below 150-200 (20) MeV : evaluated data libraries but not all isotopes up to 200 MeV

# Models for spallation reactions

Two step mechanism  
(Serber 1947)



➤ **Intra-Nuclear Cascade**  
sequence of independent  $N-N$  collisions

$$\lambda_{\text{de Broglie}} = \hbar c/p \ll \lambda \text{ mean free path}$$

fast process ( $\approx 30 \text{ fm/c}$ )

=> Excited (thermalised) remnant

➤ **De-excitation by evaporation or fission**

statistical models

slow process ( hundreds of fm/c)

➤ **Sometimes pre-equilibrium stage in-between**

→ More sophisticated models as QMD, BUU, VUU... now begin to be envisaged for implementation into high-energy transport codes

# Models for spallation reactions

## Intra-Nuclear Cascade

- Determines the number and direction of the HE particles
  - shielding against energetic neutrons
  - inter-nuclear cascade propagation
    - for Pb, INC neutrons = 15% but carry 80% of the energy
- Determines initial conditions for de-excitation
  - ◆ Excitation energy
  - ◆ Z, A of the pre-fragment
  - ◆ Angular momentum

## De-excitation

- competition between the different channels, especially at high excitation energies
  - Residue production
  - Gas production

# Results obtained during the last years

- Large amount of high quality data collected
  - Neutron and light charged particle production, isotopic residue distributions, excitation functions
- ≈ HINDAS FP5 and EUROTRANS/NUDATRA FP6 projects
- Improvement of nuclear models
  - INCL4/ABLA tested against all the available data with the same set of parameters (A.Boudard et al., PR C66 (2002) 044615)
  - also FLUKA and CEM
- Implementation of INCL4/ABLA and CEM into MCNPX, BIC and INCL4/ABLA now in GEANT4, JQMD in PHITS...

# Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions (Trieste, February 2008)

## Goals

- To bring together experts on spallation models
- To understand in depth, the physics of INC, QMD models and de-excitation models
- To define an agreed set of experimental data to be used for the benchmarking of the models
- To define the specifications of the benchmark
  - Model presentations
  - Recent experimental data



The Abdus Salam  
International Centre for Theoretical Physics



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

4 - 8 February 2008  
(Miranare, Trieste, Italy)

The International Atomic Energy Agency (IAEA) together with the Abdus Salam International Centre for Theoretical Physics (ICTP), will organize an *Advanced Workshop on Model Codes for Spallation Reactions* which will be held at the ICTP, Trieste, Italy, from 4 - 8 February 2008.

Spallation reactions play an important role in a wide domain of applications ranging from intense neutron sources for condensed matter and material studies, accelerator-driven sub-critical reactors for the transmutation of nuclear waste and rare isotope production to astrophysics, simulation of detector set-ups in nuclear and particle physics experiments, and radiation protection. In particular, the model codes for spallation reactions are needed. These are high-energy transport codes in which elementary cross-sections and characteristics of all the reaction products are taken from existing experimental library data or, when experimental data are missing, calculated using nuclear model codes as event generators. Those are generally Monte-Carlo implementations of Intra-Nuclear Cascade (INC) models or Quantum Molecular Dynamics (QMD) models followed by de-excitation (principally evaporation/fission) models. It is of great importance to validate abilities of the various codes to predict reliably, with a known uncertainty, the different quantities relevant for applications.

**PURPOSE:** This Workshop will facilitate experts and competent practitioners to better understand the physical basis, approximations, strengths and weaknesses of the currently used spallation codes. Presentation of relevant basic experimental data with emphasis on accuracies, detector efficiencies, filters and thresholds will create basis for code validation and inter-comparison. Specifically the workshop will help:

- \* To understand in depth, the physics of INC, QMD models and de-excitation models to point out the reasons of their respective successes or deficiencies;
- \* To define an agreed set of experimental data to be used in validation and inter-comparison of the models;
- \* To promote the exchange of information among researchers in the field;
- \* To identify areas of international cooperation in the field.

The agreed set of experimental data will be proposed as an international benchmark and reviewed by experts in a follow-up activity.

**PARTICIPATION:** Experts, young scientists, and Ph.D. students from all countries which are members of the United Nations, UNESCO or IAEA may attend the advanced workshop. As it will be conducted in English, participants should have an adequate working knowledge of this language. Although the main purpose of the centre is to help research workers from developing countries, through a programme of training activities within a framework of international cooperation, a limited number of young scientists, Ph.D. students, and post-doctoral scientists from developed countries are also welcome to attend this Workshop.

As a rule, travel and subsistence expenses of the participants should be borne by the home institution. Every effort should be made by candidates to secure support for their fare (or at least half-fare). However, limited funds are available for some participants, who are nationals of, and working in, a developing country. Preference will be given to qualified candidates not more than 45 years old. Such support is available only for those who attend the entire activity. There is no registration fee.

**Requests for Participation:** The "Request for Participation" form is obtainable via Web server: <http://agenda.ictp.it/smr.php?1930>. It should be completed, signed and returned by using only one of the following ways:

If sending an application by e-mail to: [smr1930@ictp.it](mailto:smr1930@ictp.it) please save and send file attachments in either PDF (preferably) or RTF zipped or DOC format.

If sending an application form by regular mail or courier it should be posted to:  
Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions  
(smr1930 c/o Ms. Patricia Wardell)  
the Abdus Salam International Centre for Theoretical Physics  
Strada Costiera 11  
34014 Trieste, Italy (recent photograph & signature of the candidate are compulsory)

**ACTIVITY SECRETARIAT:** Telephone: +39-040-2240576      Telefax: +39-040-2240585  
E-mail: [smr1930@ictp.it](mailto:smr1930@ictp.it)      ICTP Home Page: <http://www.ictp.it/>

Trieste, September 2007



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(Soreq NRC, Yavne, Israel)

**LOCAL ORGANIZER:**  
C. TUNIZ  
(ICTP, Trieste, Italy)

**TOPICS:**  
INC Models  
QMD and BUU Models  
De-Excitation Models  
Spallation reaction data for validation of models  
Model inter-comparison methods

**DEADLINE**  
for requesting participation  
**2 NOVEMBER 2007**



# Trieste workshop: 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)

# Benchmark of Spallation Models

## Objectives

- 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.

## Organizing Committee

- Detlef Filges, Forschungszentrum Jülich, Germany
- Sylvie Leray, CEA Saclay, France
- Gunter Mank, IAEA Vienna, Austria
- Yair Yariv, Soreq NRC, Israel
- Alberto Mengoni, IAEA Vienna, Austria (Scientific Officer)

## Benchmark Website

[www-nds.iaea.org/spallations](http://www-nds.iaea.org/spallations)

# Specifications

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

why 20 MeV?

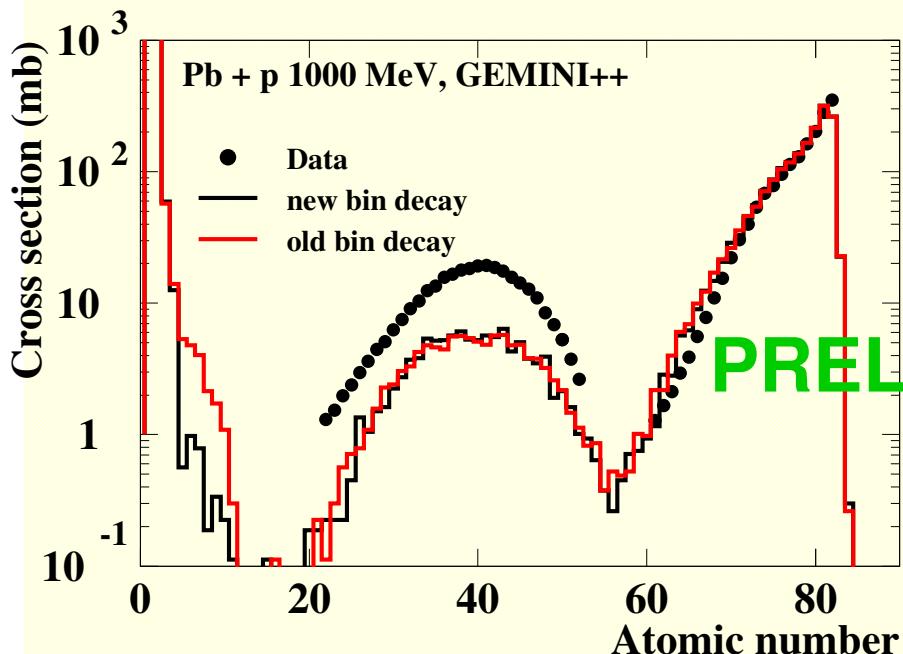
- 20-150 MeV libraries not available for all isotopes
- for residue production below 150 MeV
- to calculate correlations between particles

# Specifications of the intercomparison

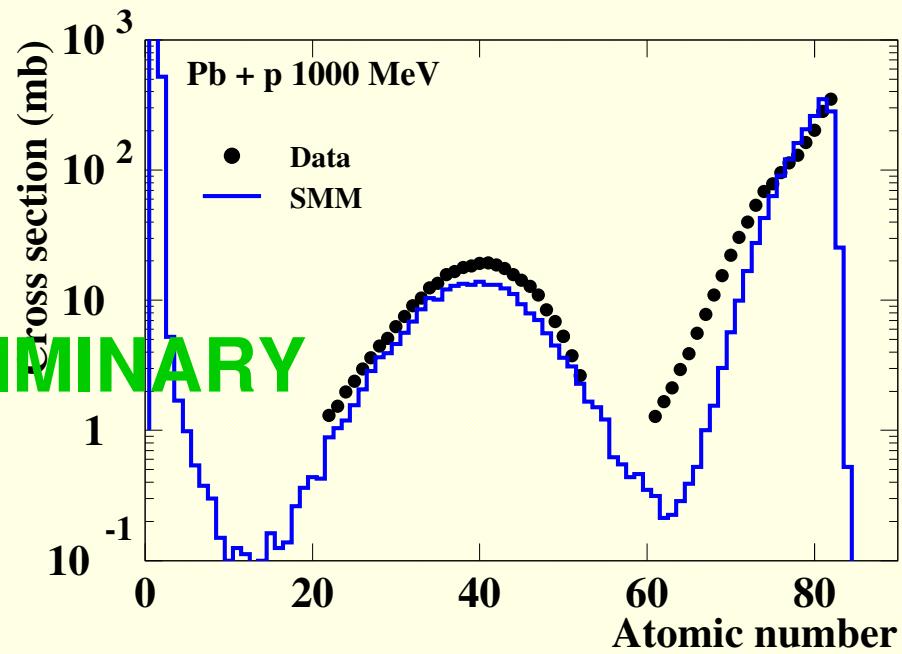
- Participants should be able to treat the complete reaction mechanism
  - complete reaction description (INC/QMD + De-ex)
- Participants should calculate the whole mandatory set of experimental data
  - + additional set if they have enough time
- Participants should give a comprehensive description 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

# Specifications of the intercomparison

- Participants should be able to treat the complete reaction mechanism
  - complete reaction description (INC/QMD + De-ex)



GEMINI++ from R. Charity



SMM from A. Botvina

Coupling to INCL4: D. Mancusi (Liège)

# 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
- ↳  $\sigma_{\text{inv}}$
- ↳ fission barriers
- ↳ fission fragment distributions
- ↳ ...

# Additional information on the calculation

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

→ To understand the reasons for success or deficiency

## Choice of experimental data

- Presentations on recent experimental data
  - NESSI and PISA data on light charged particles and IMFs (F. Goldenbaum)
  - GSI residues isotopic distributions (J. Benlliure)
  - residue excitation functions (Y. Titarenko, R. Michel)
- Set of data to be used for the benchmark
  - All reaction channels
  - Restriction to a limited number of systems (mainly Fe and Pb), a few energies covering the full range

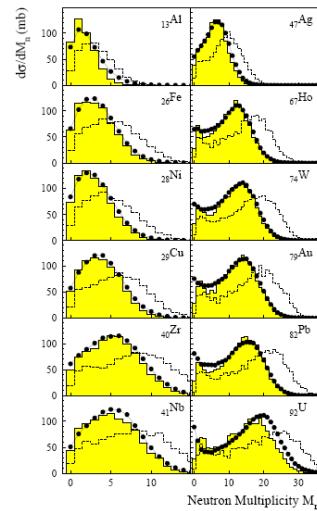
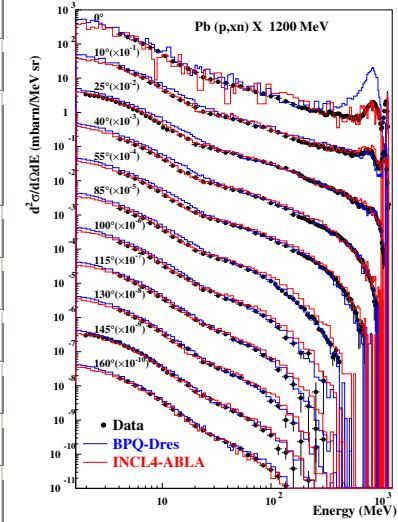
## Neutron production

### Double-differential Cross Sections

Beam	Target	Energy [MeV]	Angles [degrees]	Laboratory	Reference	Data
n	Fe	65	9.5 - 28	Univ. California, USA	E. L. Hjort et al., Phys. Rev. C 53 (1996) 237 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Fe	800	0 - 160 30 - 150	Saturne, France LANL, USA	S. Leray et al., Phys. Rev. C 65 (2002) 044621 - W.B. Amian et al., Nucl. Sci. Eng. 112 (1992) 78 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Fe	1200	0 - 160	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Fe	1600	0 - 160	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Fe	3000	15 - 150	KEK, Japan	K. Ishibashi et al., J. of Nucl. Sci. Tech. 34 (1997) 529 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	63	24 - 140	Louvain, Belgium	A. Guertin et al., Eur. Phys. J. A23 (2005) 49 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	256	8 - 150	LANL, USA	M. Meier et al., Nucl. Sci. Eng. 110 (1993) 289	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	800	0 - 160 30 - 150	Saturne, France LANL, USA	S. Leray et al., Phys. Rev. C 65 (2002) 044621 - W.B. Amian et al., Nucl. Sci. Eng. 112 (1992) 78 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	1200	0 - 160	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	1600	0 - 160	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
p	Pb	3000	15 - 150	KEK, Japan	K. Ishibashi et al., J. of Nucl. Sci. Tech. 34 (1997) 529 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>

### Multiplicity Distributions

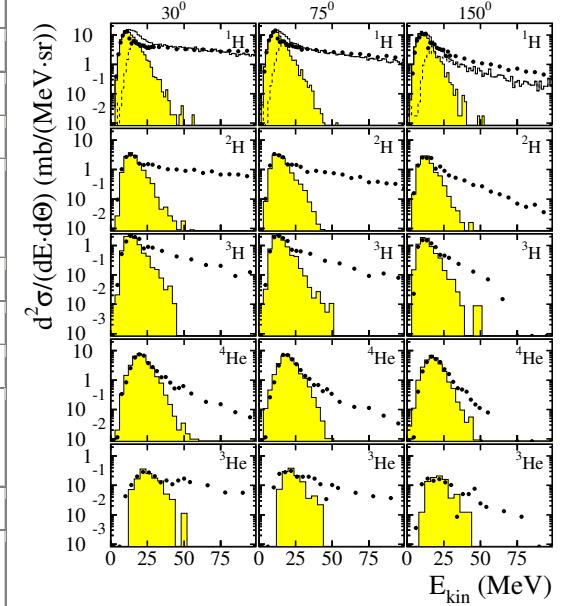
Beam	Target	Energy [MeV]	Laboratory	Reference	Data
p	Fe	800, 1200, 1600	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>
p	Fe	1200	COSY, Germany	C.-M. Herbach et al., Jülich annual report (2001) -	<a href="#">data</a>   <a href="#">figure</a>
p	Pb	800, 1200, 1600	Saturne, France	S. Leray et al., Phys. Rev. C 65 (2002) 044621 -	<a href="#">data</a>
p	Pb	1200	COSY, Germany	A. Letourneau et al., Nucl. Inst. Meth. B 170 (2000) 299 -	<a href="#">data</a>   <a href="#">figure</a>



## Light charged particle production

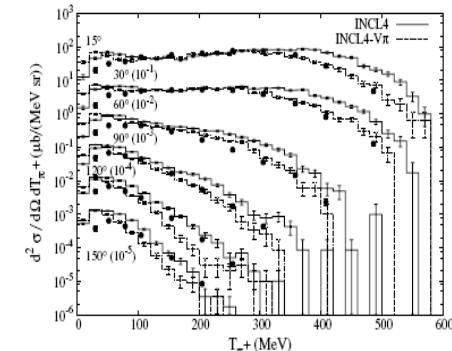
### Double-differential Cross Section

Beam	Target	Energy [MeV]	Emitted particles	Laboratory	Reference	Data
n	Bi	542	p, d, t	PSI, Switzerland	J. Franz et al., Nucl. Phys. A 510 (1990) 774 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR (p - d - t)
p	Al	160	$\alpha$	iTHEMBA, South Africa	A. Cowley et al., Phys. Rev. C 54 (1996) 778 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR
p	Fe	62	p, d, t, $^3\text{He}$ , $\alpha$	LANL, USA	F.E. Bertrand and R.W. Pelle, Phys. Rev. C 8 (1973) 1045 -	<a href="#">data</a>   <a href="#">figures</a>   EXFOR (p - d - t - $^3\text{He}$ - $\alpha$ )
p	Ni	175	p, d, t, $^3\text{He}$ , $\alpha$ p	COSY, Germany	F. Goldenbaum et al. (unpublished)	<a href="#">data</a>   <a href="#">figures</a>
					S.V. Förtsch et al., Phys. Rev. C 43 (1991) 691 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR
p	Ta	1200	p, d, t, $^3\text{He}$ , $\alpha$	COSY, Germany	C.-M. Herbach et al., Nucl. Phys. A 765 (2006) 426 -	<a href="#">data</a>   <a href="#">figure</a>
p	Au	160	$\alpha$	iTHEMBA, South Africa	A. Cowley et al., Phys. Rev. C 54 (1996) 778 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR
p	Au	1200	p, d, t, $^3\text{He}$ , $\alpha$	COSY, Germany	A. Budzanowski et al. (to be published)	<a href="#">data</a>   <a href="#">figures</a>
p	Au	2500	p, d, t, $^3\text{He}$ , $\alpha$	COSY, Germany	A. Letourneau et al., Nucl. Phys. A 712 (2002) 133 -	<a href="#">data</a>   <a href="#">figures</a>
					A. Bubak et al., Phys. Rev. C 76 (2007) 014618 -	<a href="#">data</a>   <a href="#">figures</a>
p	Pb	63	p, d, t, $^3\text{He}$ , $\alpha$	Louvain-la-Neuve, Belgium	A. Guertin et al., Eur. Phys. J. A 23 (2005) 49 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR (p - d - t - $^3\text{He}$ - $\alpha$ )
p	Pb	800	p	LANL, USA	R. Chrien et al., Phys. Rev. C 21 (1980) 1014 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR
					J.A. McGill et al., Phys. Rev. C 29 (1984) 204 -	<a href="#">data</a>   <a href="#">figure</a>   EXFOR
p	Bi	62	p, d, t, $^3\text{He}$ , $\alpha$	LANL, USA	F.E. Bertrand and R.W. Pelle, Phys. Rev. C 8 (1973) 1045 -	<a href="#">data</a>   <a href="#">figures</a>   EXFOR (p - d - t - $^3\text{He}$ - $\alpha$ )



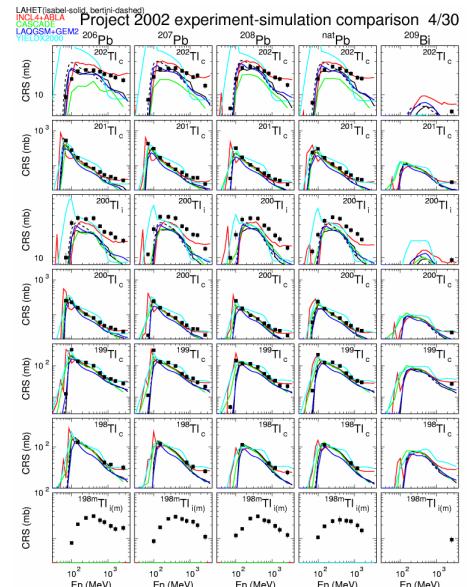
### Pion production

Beam	Target	Energy [MeV]	Emitted particles	Laboratory	Reference	Data
p	C	730	$\pi^+$ , $\pi^-$	LANL, USA	D. R. F. Cochran et al., Phys. Rev. D 6 (1972) 3085 -	<a href="#">data</a>   <a href="#">figure</a>
p	Al	730	$\pi^+$ , $\pi^-$	LANL, USA	D. R. F. Cochran et al., Phys. Rev. D 6 (1972) 3085 -	<a href="#">data</a>   <a href="#">figure</a>
p	Cu	730	$\pi^+$ , $\pi^-$	LANL, USA	D. R. F. Cochran et al., Phys. Rev. D 6 (1972) 3085 -	<a href="#">data</a>   <a href="#">figure</a>
p	Pb	730	$\pi^+$ , $\pi^-$	LANL, USA	D. R. F. Cochran et al., Phys. Rev. D 6 (1972) 3085 -	<a href="#">data</a>   <a href="#">figure</a>
p	Al	2205	$\pi^-$	KEK, Japan	H. En'yo et al., Phys. Lett. 159B (1985) 1 -	<a href="#">data</a>   <a href="#">figure</a>



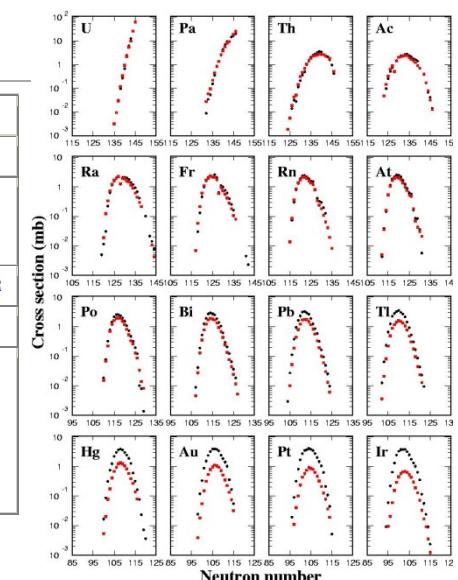
## Production cross-sections from threshold to 3 GeV (excitation functions)

Beam	Target	Energy [MeV]	Laboratory	Reference	Data
p	Fe	20 to 3000	Hannover University, Germany University of Bern, Switzerland ITEP, Russian Federation	R. Michel et al., Nucl. Sci. Tech., Supplement 2 (2002) 242 - K. Ammon, I. Leya et al., Nucl. Instr. and Meth. B 266 (2008) 2 - R. Michel et al., Nucl. Instr. and Meth. B 103 (1995) 183 -; Th. Schiekel, R. Michel et al., Nucl. Instr. and Meth. B 114 (1996) 91 -; R. Michel et al., Nucl. Instr. and Meth. B 129 (1997) 153 - Titarenko (soon, october 2008?)	<a href="#">data</a>   <a href="#">figure</a> <a href="#">data</a>   <a href="#">figure</a>  <a href="#">data</a>   <a href="#">figure</a>  <a href="#">data</a>   <a href="#">figure</a>
p	Pb	20 to 3000	ITEP, Russian Federation ETH Zürich, Switzerland Hannover University, Germany	Y. E. Titarenko et al., Nucl. Instr. and Meth. A562 (2006) 801 - M. Gloris et al., Nucl. Instr. and Meth. A463 (2001) 593 - I. Leya et al., Nucl. Instr. and Meth. B229 (2005) 1 -	<a href="#">data</a>   <a href="#">figure</a> <a href="#">data</a>   <a href="#">figure</a> <a href="#">data</a>   <a href="#">figure</a>



## Isotopic distribution cross-sections in inverse kinematics

Beam	Target	Energy [A MeV]	Laboratory	Reference	Data
Fe	H	300	GSI, Germany	C. Villagrasa-Canton et al., Phys. Rev. C 75 (2007) 044603 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">GSI</a>
Fe	H	1000	GSI, Germany	C. Villagrasa-Canton et al., Phys. Rev. C 75 (2007) 044603 - P. Napolitani et al., Phys. Rev. C 70 (2004) 054607 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">GSI</a>
Pb	H	500	GSI, Germany	L. Audouin et al., Nucl. Phys. A768 (2006) 1 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">EXFOR</a>
Pb	H	1000	GSI, Germany	T. Enqvist et al., Nucl. Phys. A686 (2001) 481 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">GSI</a>
U	H	1000	GSI, Germany	J. Taieb et al., Nucl. Phys. A 724 (2003) 413 - M. Bernas et al., Nucl. Phys. A765 (2006) 197 - M. Bernas et al., Nucl. Phys. A 725 (2003) 213 - M. V. Ricciardi et al., Phys. Rev. C 73 (2006) 014607 -	<a href="#">data</a>   <a href="#">figure</a>   <a href="#">GSI</a>



# Benchmark of Spallation Models

## List of participating models

- CEM0303 (A. Gudima)
- CEM0302 (S. Mashnik)
- PHITS-jam (N. Matsuda)
- PHITS-Bertini (N. Matsuda)
- PHITS-JQMD (N. Matsuda)
- Cascade04 (H. Kumawat)
- Isabel-SMM (Y.Yariv / A. Botvina / D. Mancusi)
- Isabel-Gemini (Y.Yariv / R. Charity / D. Mancusi)
- Isabel-ABLA07\* (Y.Yariv / A. Kelic / V. Ricciardi / D. Mancusi)
- Geant4-Bertini (D. Wright)
- Geant4-BIC (D. Wright)
- Cascade-ASF (A. Konobeyev)
- INCL4.5-SMM\* (J. Cugnon / A. Boudard / A. Botvina / D. Mancusi)
- INCL4.5-Gemini\* (J. Cugnon / A. Boudard / R. Charity / D. Mancusi)
- INCL4.5-ABLA07\* (J. Cugnon / A. Boudard / A. Kelic / V. Ricciardi / D. Mancusi)
- FLUKA\* (A. Ferrari)

\* Not yet received

# AccApp09 Satellite Meeting Nuclear Spallation Reactions

## → Presentations by the participants of their results

- J. Cugnon: [Results obtained with INCL4](#)
- Y. Yariv: [Results obtained with ISABEL](#)
- M.V. Ricciardi: [Results obtained with ABLA07](#)
- D. Mancusi: [Comparison between various de-excitation models](#)
- S. Kailas: [Results obtained with CASCADE-0.4](#)
- A. Gudima: [Results obtained with CEM03](#)
- J.M. Quesada-Molina: [Results obtained with GEANT4](#)
- N. Matsuda: [Results obtained with nuclear models of PHITS](#)

## → M. Khandaker: Presentation of the tools and first results

## → Discussions

- Benchmark strategy, definition of the figures of merit
- Conclusions and plans for the future