Microscopic description of proton-induced spallation reactions with the CoMD (Constrained Molecular Dynamics) model

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Outline

- Motivation: applications of spallation reactions
- Recent Literature of spallation
- Description of the theoretical CoMD model
- Comparison between experimental & theoretical preliminary results
- Future work plan
- Summary and conclusions

Applications of spallation

- Accelerator- driven systems (ADS)
- Energy amplification
- Transmutation of nuclear waste

- Sources of spallation neutrons

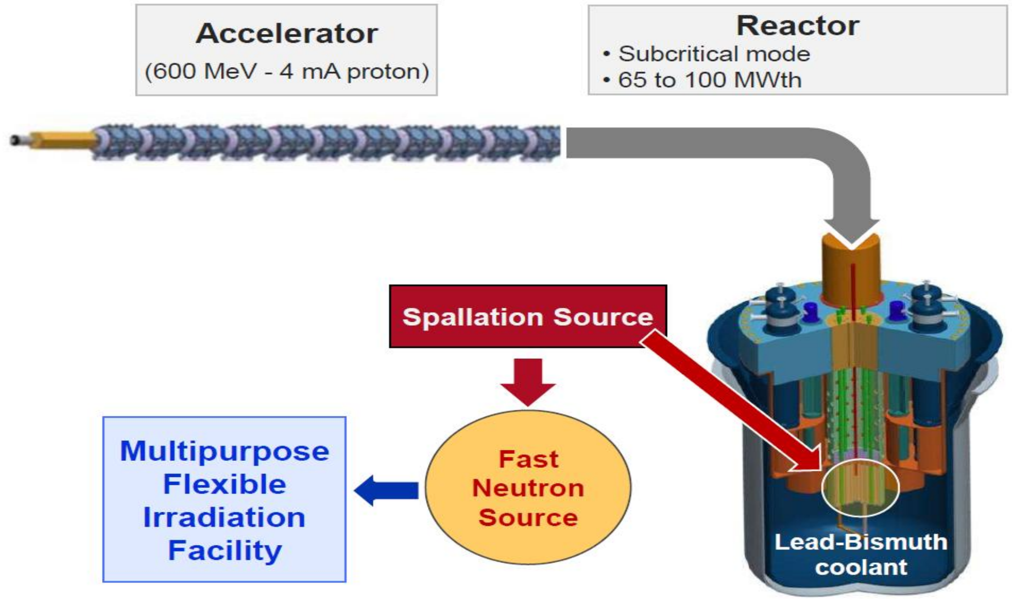
- Production of rare isotopes (ISOL facilities)

- Astrophysics (reactions induced by cosmic rays in interstellar medium)

Accelerator driven system (ADS)

- High energy proton beam bombards a heavy metal target (Pb, Th, U)
- A large number of neutrons is produced by spallation &
- Directed to the subcritical core (e.g. Th, U)

MYRRHA research reactor in Belgian Nuclear Research Centre



Accelerator Transmutation of Waste (ATW)

- ATW: a variant of ADS
- Instead of fissile fuel there is a blanket containing the waste
- Nuclear waste (i.e. spent nuclear fuel): significant part is long-lived actinides (Np, Am, Cm)
- Transmutation of long- lived radioisotopes into stable or short-lived elements
- Possibility of safe storage

Element	Half-life (years)	Type	Percent of Fuel
Sr-90	~30	Fission Product (FP)	0.04
Cs-137	~30	FP	0.09
Tc-99	$\sim 10^6$	FP	0.09
I-129	$\sim 10^7$	FP	0.03
Np-237	2.0×10^6	Transuranic (TRU)	0.05
Am-241	400	TRU	0.01

Spallation neutron sources: Applications and Facilities

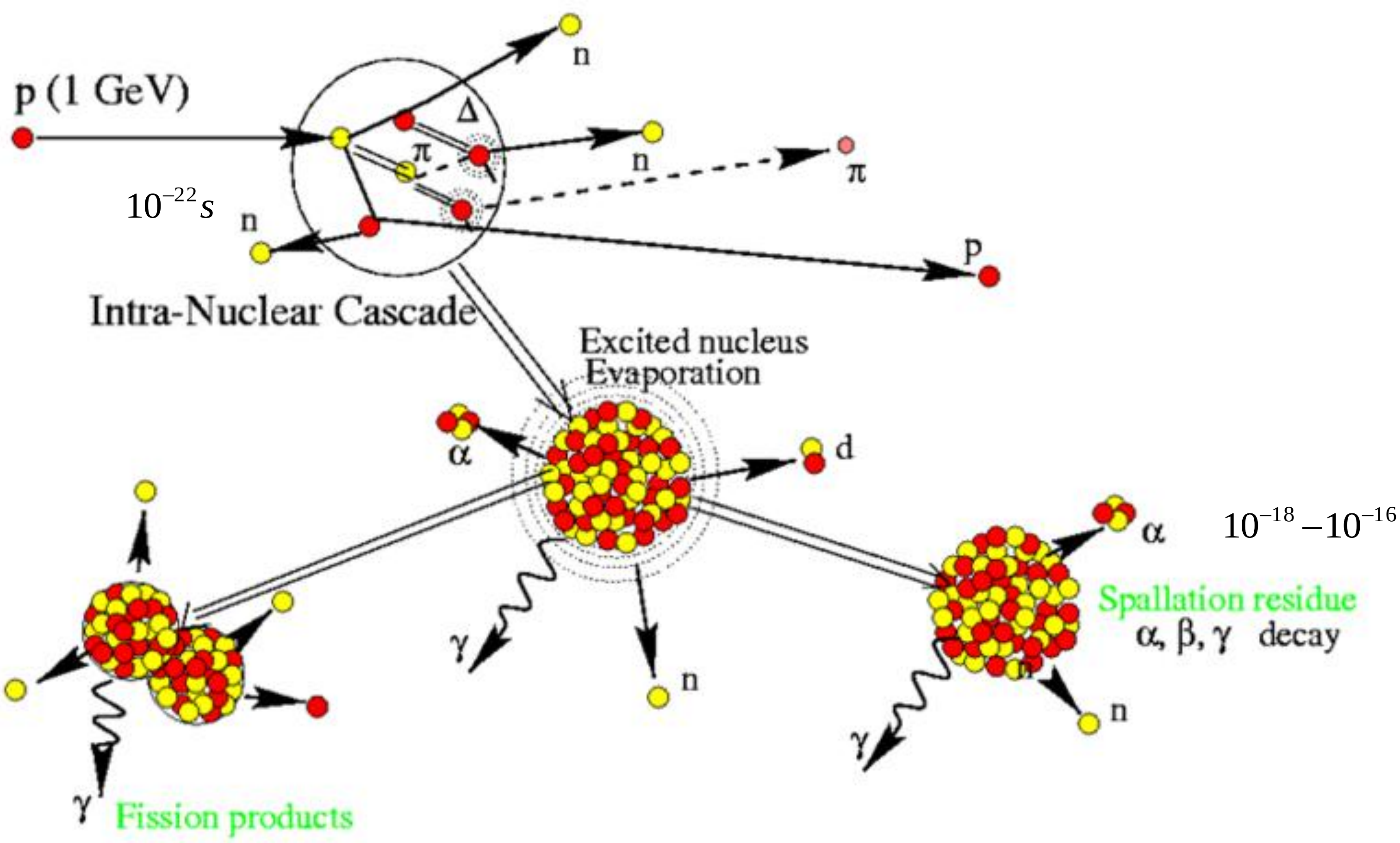
- Neutrons as probe in condensed matter science

  (e.g. gain new insights into atomic disordering in complex metal oxides)

- Biology:
- Understanding new theories in Cellular Membrane organization (presence and formation of nanoscale lipid patches)
- simulation of lipid bilayer or cell membrane (understanding how viruses invade healthy cells)

- ESS, Lund, Sweden
- SINQ, Switzerland
- GEMS, Germany
- ISIS, UK
- SNS, Oak Ridge, USA
- LANSCE, Los Alamos, USA
- J-PARC, Japan

Spallation reaction mechanism



Recent Literature of spallation

M. V. Ricciardi et al., Phys. Rev. C 73, 014607 (2006)

- Experimental study of ^{238}U (1GeV/u) + p at the FRS in GSI
- Formation of 254 isotopes in the range 7 ≤ Z ≤ 37
- Statistical code ABRABLA (abrasion- ablation) used for comparisons

J. L. Rodriguez-Sanchez,J. Benlliure,et al. Phys. Rev. C 90, 064606 (2014)

- Measurement of fission cross sections in ^{208}Pb + p at 370, 500, 650 MeV/u at GSI
- Description with INCL4.6 & ABLA07

Y. Ayyad, J. Benlliure et al., Physical Review C 89, 054610 (2014)

- Measurement of total fission cross sections at 300 – 1000MeV
- Experimental & theoretical study of ^{181}Ta + p (inverse kinematics) in GSI
- Description of reaction with intranuclear cascade models (INCL4.6 (Liege') and ISABEL) & deexcitation codes (ABLA07 and GEMINI++)

Recent Literature of spallation

A. A. Kotov et al., Physical Review C 74, 034605 (2006)

- Measurement of fission cross sections ^{nat}Pb, ^{209}Bi, ^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{237}Np & ^{239}Pu in energy range 200-1000 MeV
- Detection of 2 fission fragments by 2 (PPAC)

J. L. Rodriguez- Sanchez, J. Benlliure et al., Physical Review C 91, 064616 (2015)

- ^{208}Pb (500 MeV/u) + p performed at GSI
- Measurement of isotopic cross sections, velocities of ff (Z = 27 to Z = 52), mass yields
- Identification of Z with MUSIC
- Comparison of results with INCL4.6 + ABLA07 code

Description of the theoretical CoMD model

CoMD: Quantum Molecular Dynamics Model (Semiclassical)

- The nucleons considered as gaussian wavepackets
- Phenomenological interaction N-N (Skyrme effective interaction)
- Asymmetry potential N-N depending on the nuclear density
- Application of Pauli Principle through appropriate restriction in the phase space
- Recognition of fragment formation (R_{N-N} < 3.0 fm)
- Simulation of successive events (**Monte Carlo approach**)

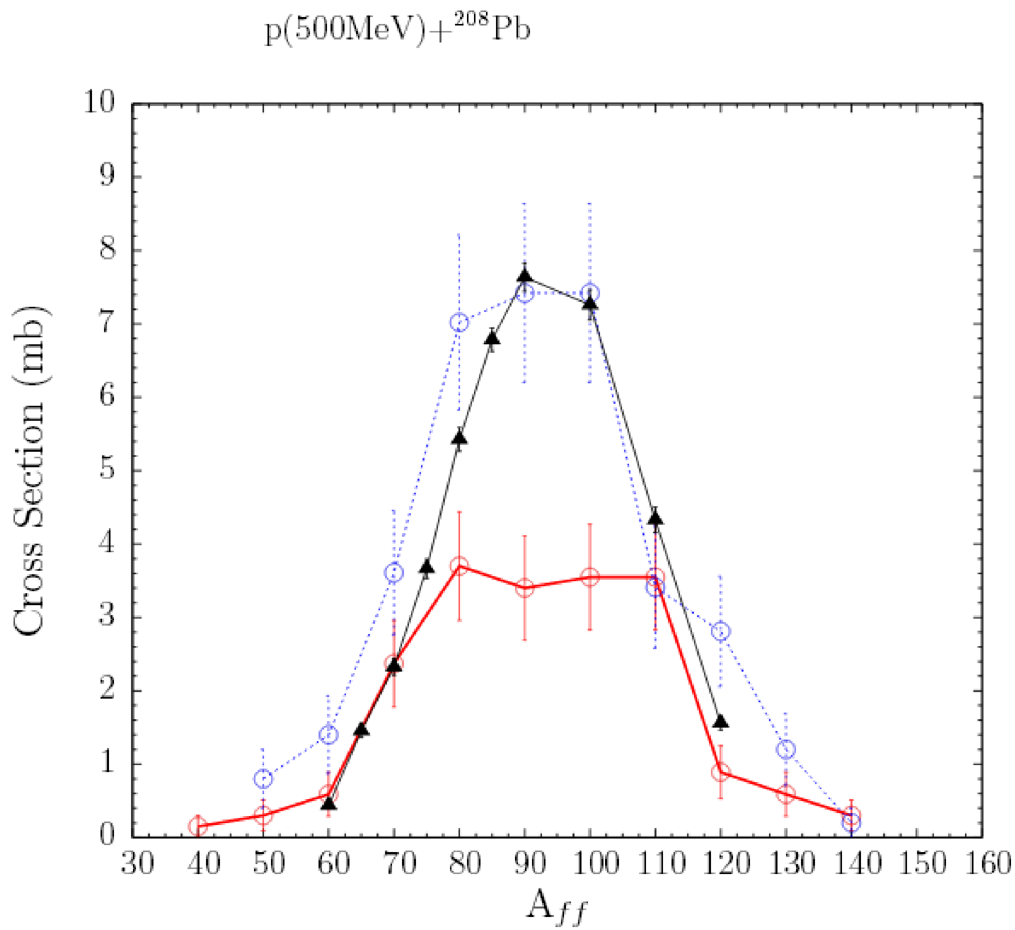
Comparison between theoretical and experimental results: p(500 MeV) + ^{208}Pb

CoMD calculations

Red line: standard $V_{sym} \sim \rho$

Blue line: soft $V_{sym} \sim \sqrt{\rho}$

Black points: experiment



CoMD calculations agree very well with the experimental data

Our calculations indicate symmetric fission: shell effects not included

J. L. Rodriguez- Sanchez, J. Benlliure et al., Phys. Rev.C 91, 064616 (2015)

Comparison between theoretical and experimental results: p (500 MeV, 1000MeV) + ^{208}Pb

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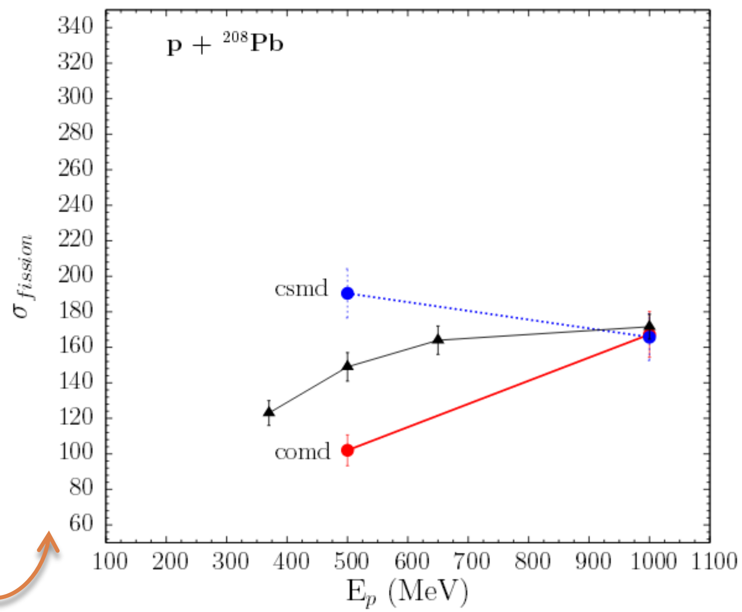

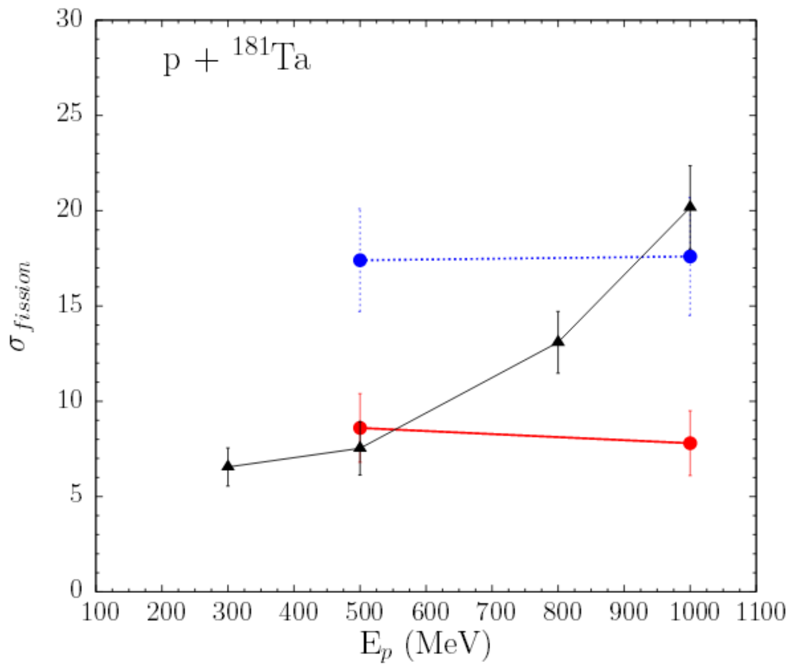

J. L. Rodriguez-Sanchez,J. Benlliure,et al. Phys. Rev. C 90, 064606 (2014)

Y. Ayyad, J. Benlliure et al., Physical Review C 89, 054610 (2014)

Comparison between theoretical and experimental results: p(100- 1000MeV) + ^{238}U

CoMD calculations

Red line: standard $V_{sym} \sim \rho$

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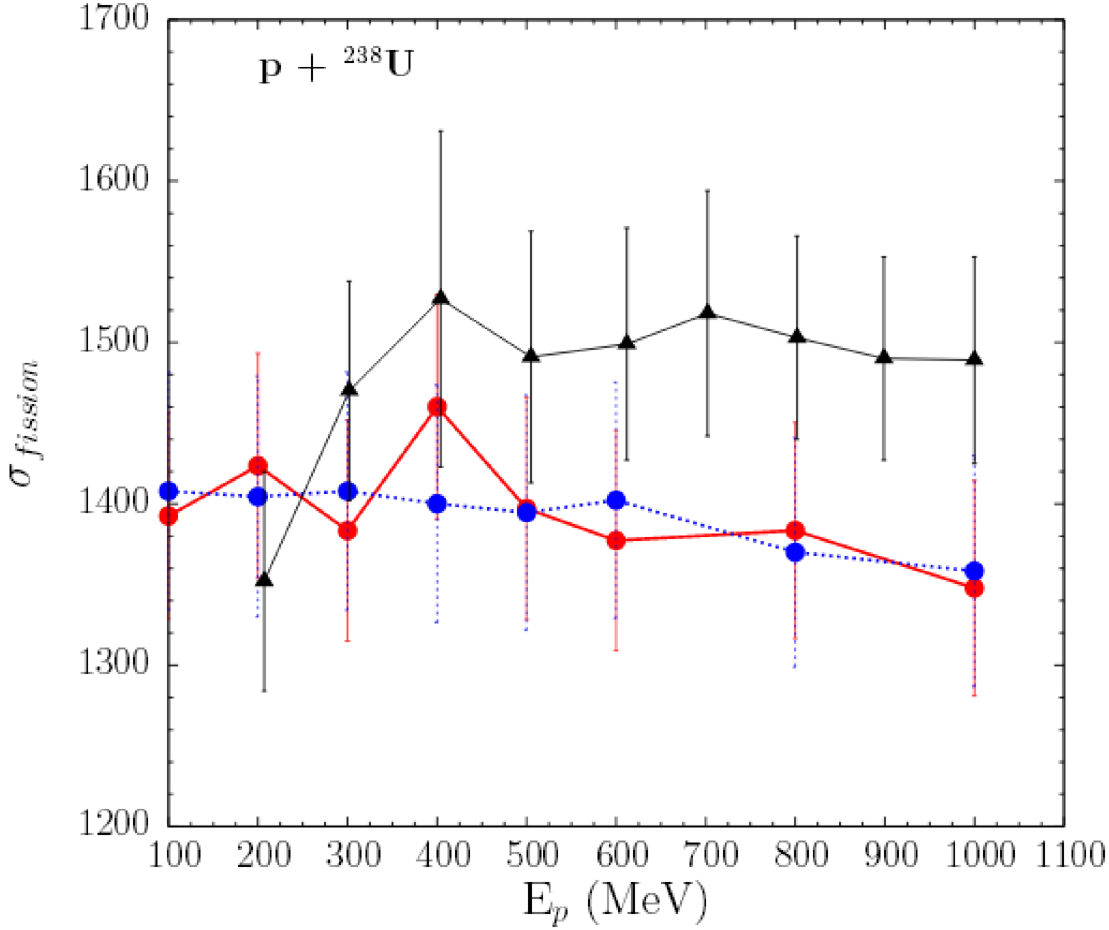
Black points: experiment



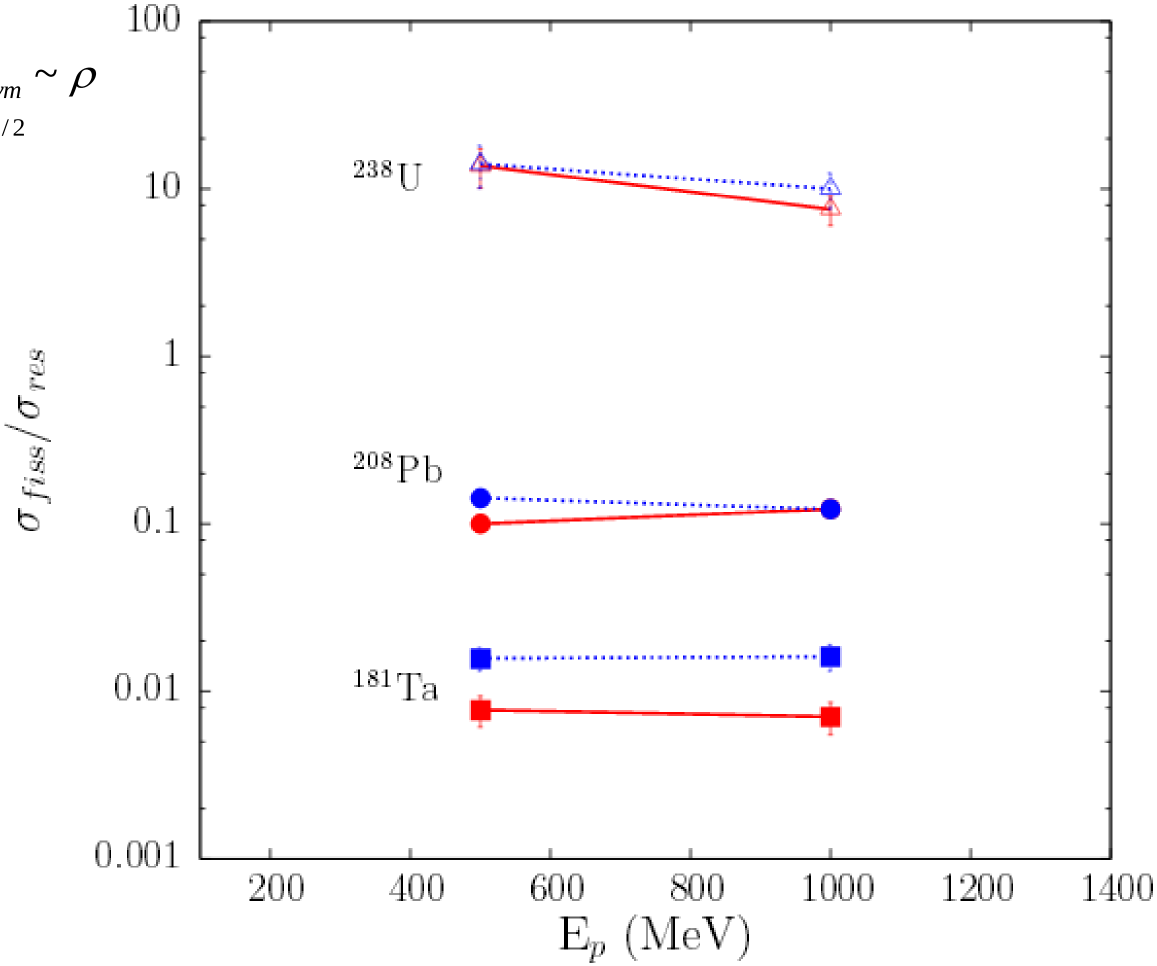
M. V. Ricciardi et al., Phys. Rev. C 73, 014607 (2006)

Fission cross section/residue cross section

CoMD calculations

Red line: standard $V_{sym} \sim \rho$

Blue line: soft $V_{sym} \sim \rho^{1/2}$



High fissility

Modest fissility

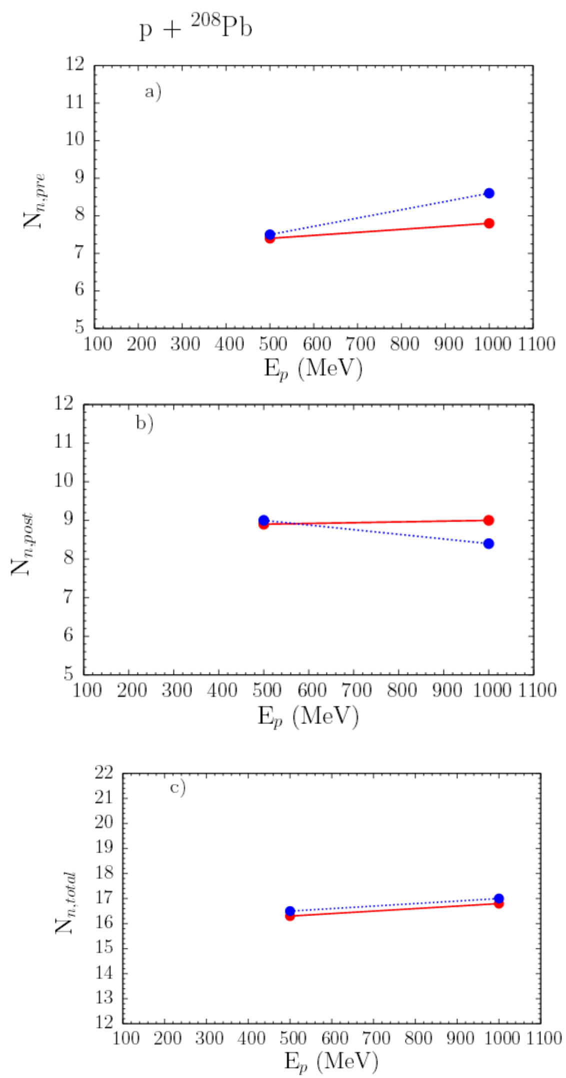
Low fissility

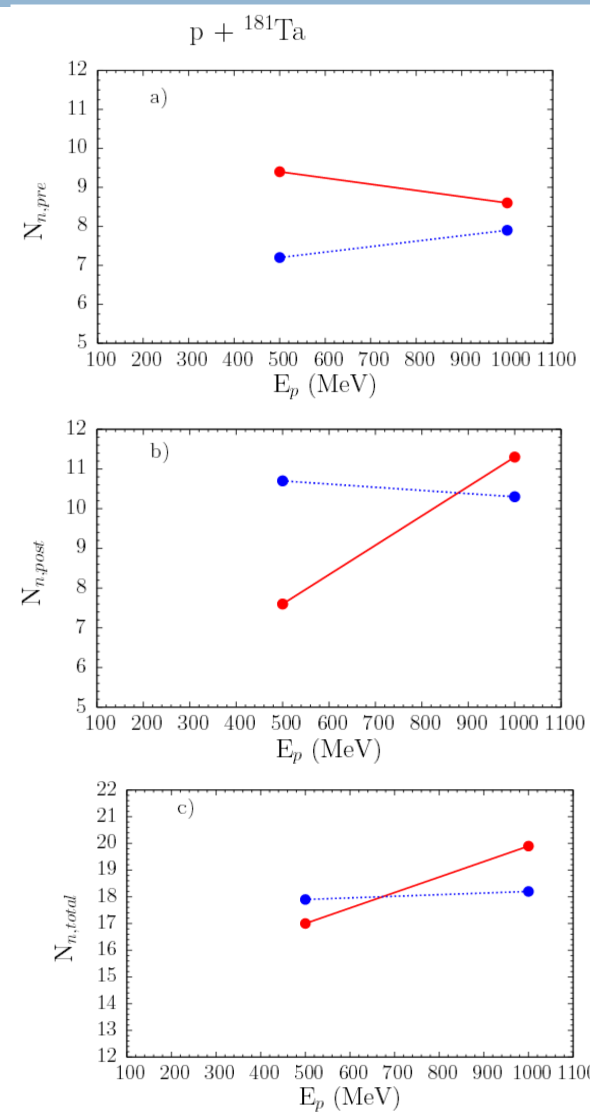
Neutron multiplicity

CoMD calculations

Red line: standard $V_{sym} \sim \rho$

Blue line: soft $V_{sym} \sim \rho^{1/2}$





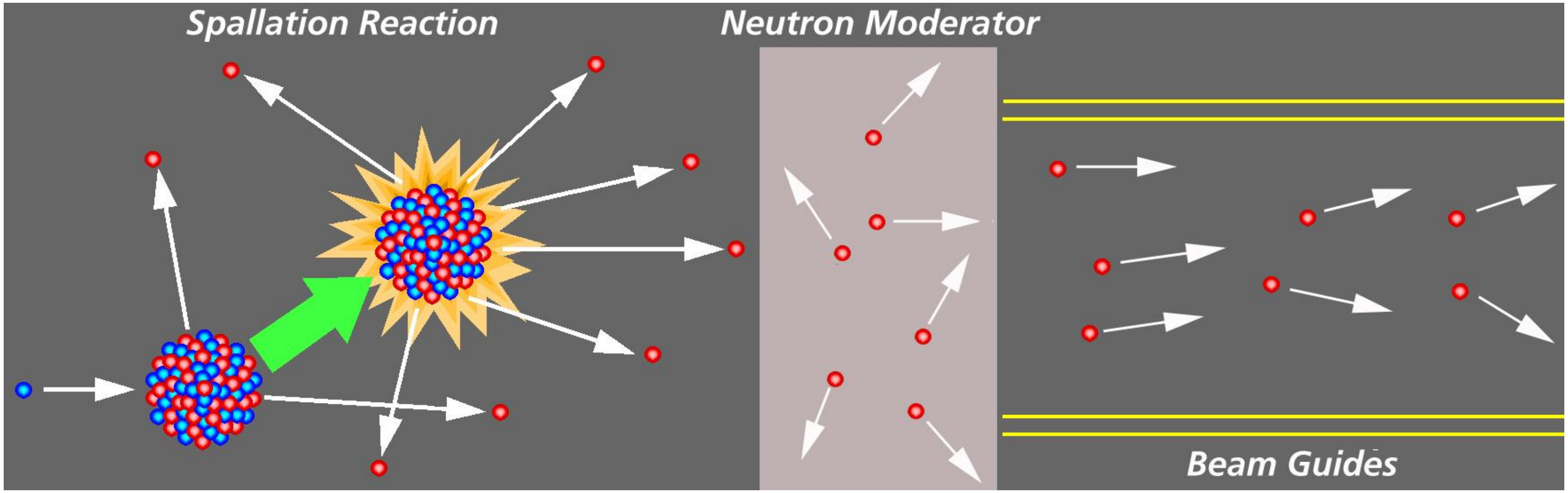
Spallation neutron multiplicities:15 -20 neutrons

Future work plan

- Systematic study of spallation observables
  - Mass yield curves
  - Energy distributions
  - Fission time scale
  - Pre-scission, post-scission, total nucleon emission (especially neutrons)
  - Heavy-residue/fission-fragment production (residue data necessary)

- Contribution of the present spallation systematics to practical applications (e.g. sytematics of spallation neutrons)

Thank you!



Neutron multiplicity

CoMD calculations

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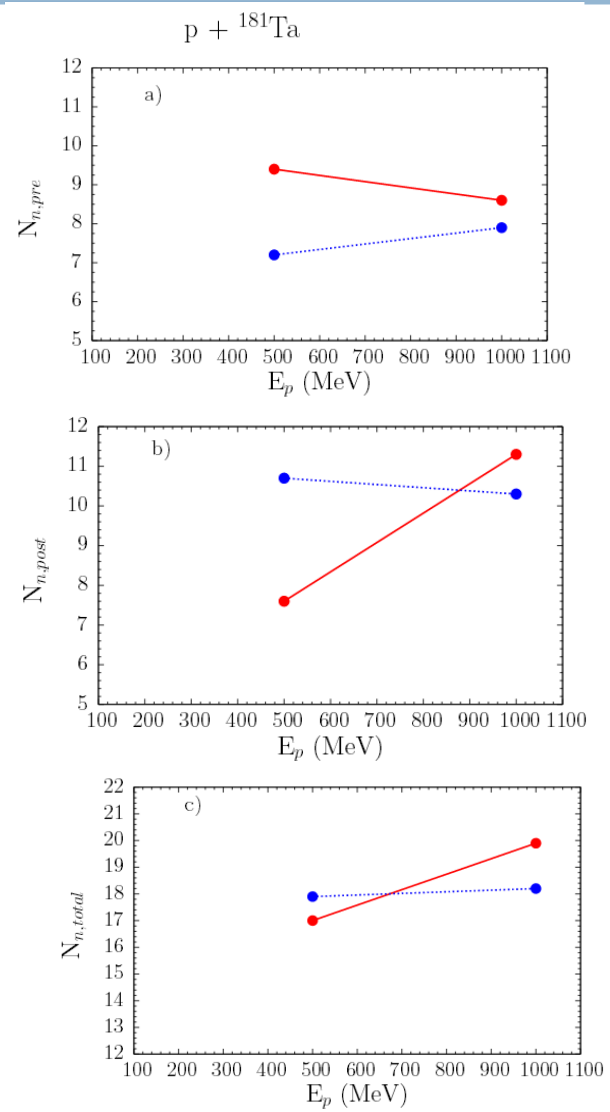

Comparison between theoretical and experimental results: p (500 MeV, 1000MeV) + ^{181}Ta

CoMD calculations

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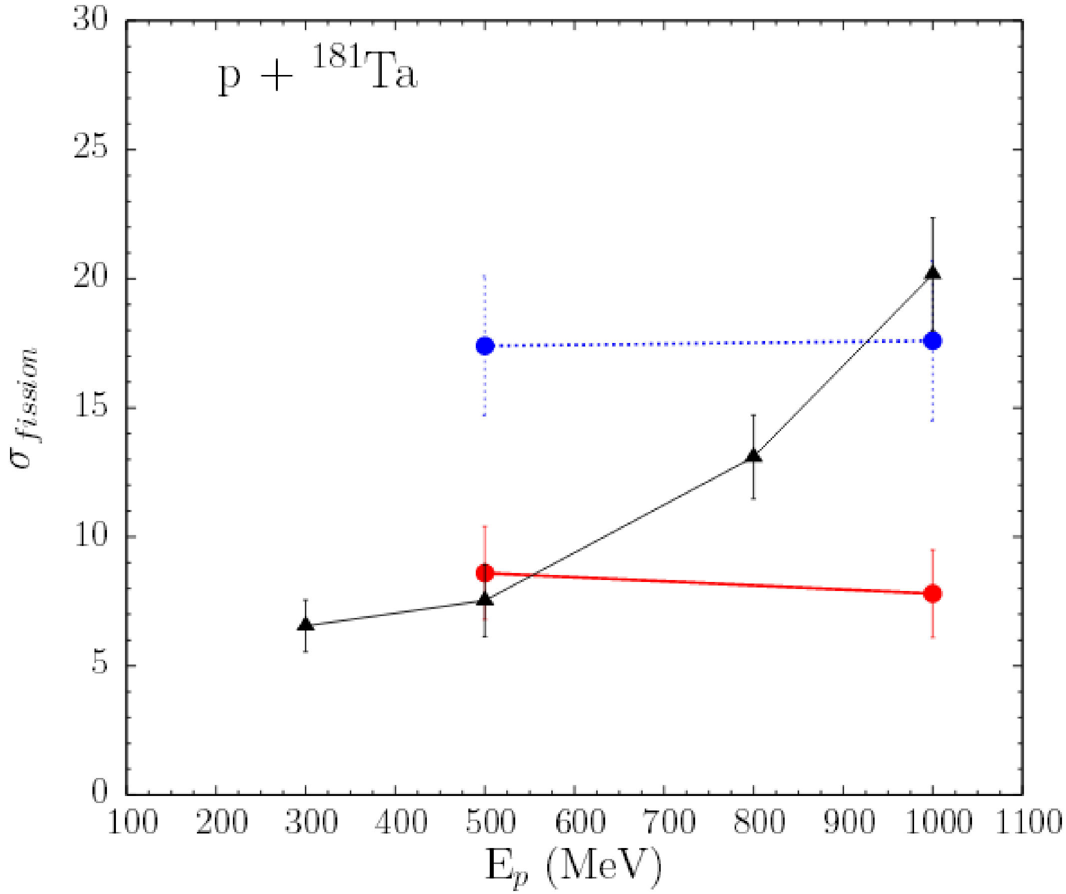


Y. Ayyad, J. Benlliure et al., Physical Review C 89, 054610 (2014)

Fission neutrons

- Fission: $n + {}^{235}U = n + n + \text{fragments}$

Sustain chain reaction

200 MeV/n

available → moderated by

↓

D_2O (H_2O)

Accelerator Transmutation of Waste (ATW)

- A significant proportion of wastes in used nuclear fuel is long- lived actinides (Np, Am, Cm)
- Following neutron capture heavy isotopes fission producing energy
- Bombardment of waste with intense neutron flux produced from *spallation*
  - Heavier elements fission into less dangerous species
  - Lighter elements are converted through neutron absorption

Spallation reactions

- *Spallation* is a nuclear reaction in which a high energy projectile interacts with a heavy nucleus
- High energy projectile interacts with target nucleons individually, as nucleon-nucleon collisions, inducing a succession of binary collisions on a time scale 10^{-22} s. This is called ***intra- nuclear cascade***
- Energetic neutrons, protons, pions and light particles are being emitted and others deposit their kinetic energy in the nucleus resulting in an excited residual in thermodynamical equilibrium, with E^* few MeV/nucleon
- **Equilibrium stage**: de-excitation of residual nucleus through
- evaporation(n, p, d, a) on time scale $10^{-18} - 10^{-16}$
- fission into 2 fragments
- Fragmentation (residual nucleus breaks up fast into a large number of IMF's

Spallation neutrons

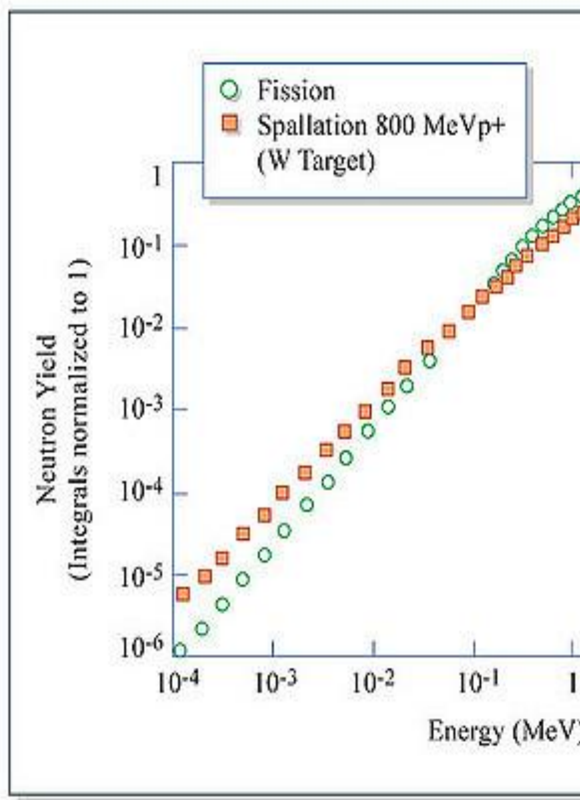
- Spallation: 20 neutrons/GeV proton are created

  Fission: 2.5 neutrons/fission event

- Spallation: p + heavy nucleus = 20 n + fragments

  1GeV *e.g. W, Pb, U*

  23 MeV/n



- Number of neutrons ∝ beam energy & mass number of target
- Spallation ***n*** energy: from tens of keV up to incident proton energy, maximum 2 MeV
- Fission ***n*** energy: from thermal energies up to 10 MeV, maximum 1 MeV