A Reevaluation of Radiation Damage Cross Sections

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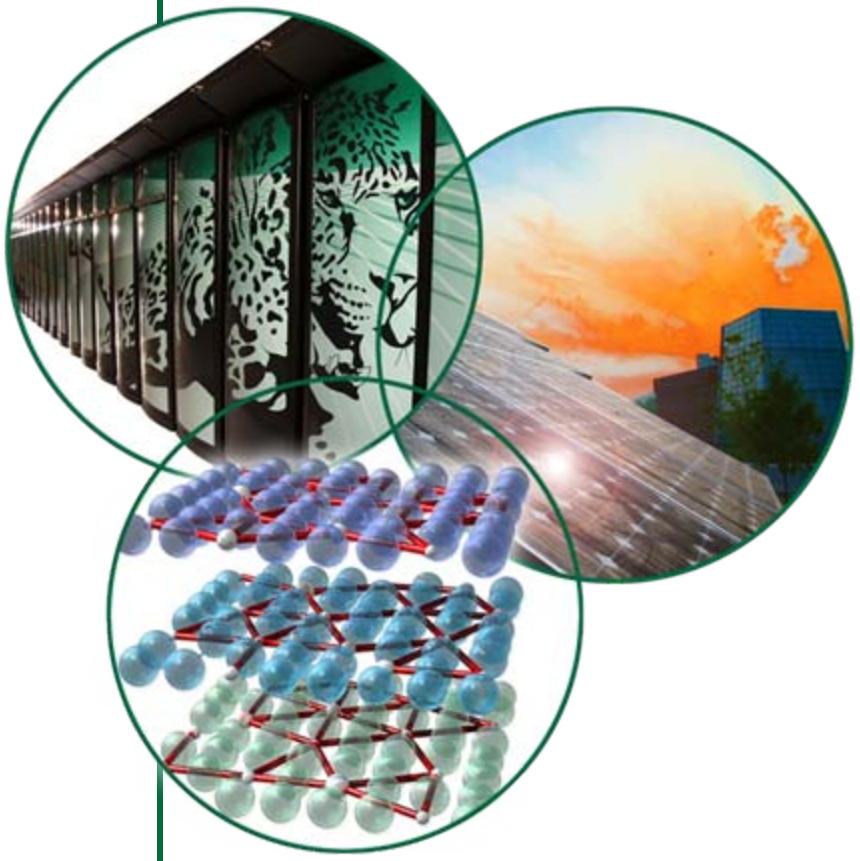

10th International Workshop on Spallation Materials Technology (IWSMT-10)
Beijing, China Oct. 18-22, 2010

U.S. DEPARTMENT OF ENERGY

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Contents

NCSU Radiation damage database -1

- Developed at NCSU in 2004, sponsored by LANL
- Cross sections (1 < p E < 3200 MeV and 1E-8 < n E < 3200 MeV)
  - damage energy and displacement
  - helium production
  - hydrogen production
  - heavier transmutation products
- Intranuclear cascade models (INC)
  - Bertini, ISABEL and CEM2k
- Evaluated data sources
  - SPECTER (ENDF-5), ENDF-6 & LA150
- Experimental results (mainly for He and H CS)

NCSU Radiation damage database -2

- Elemental targets
  - Group 1: $_{12}$Mg, $_{13}$Al, $_{14}$Si
  - Group 2: $_{22}$Ti, $_{23}$V, $_{24}$Cr, $_{25}$Mn, $_{26}$Fe, $_{27}$Co, $_{28}$Ni, $_{29}$Cu
  - Group 3: $_{40}$Zr, $_{41}$Nb, $_{42}$Mo, $_{47}$Ag, $_{50}$Sn
  - Group 4: $_{73}$Ta, $_{74}$W, $_{79}$Au, $_{80}$Hg, $_{82}$Pb, $_{83}$Bi
  - Group 5: $_{92}$U
- Alloys
  - AlMg3 (Al-2.72Mg-0.35Mn-0.25Fe)
  - EP823 (Fe-12Cr-1.8Si-0.9Ni-0.7Mo-0.7Mn)
  - Eurofer97 (Fe-9Cr-1.1W-0.4Mn)
  - F82H (Fe-7.9Cr-2.0W-0.2V)
  - HT9 (Fe-11.8Cr-1.0Mo-0.6Ni-0.5Mn)
  - SS316L (Fe-17.5Cr-12.2Ni-2.5Mo-1.8Mn)
  - T91 (Fe-8.6Cr-1.0Mn-0.2Ni)
  - Zr-2 (Zr-1.36Sn-0.17Fe-0.13O-0.11Cr-0.07Ni)

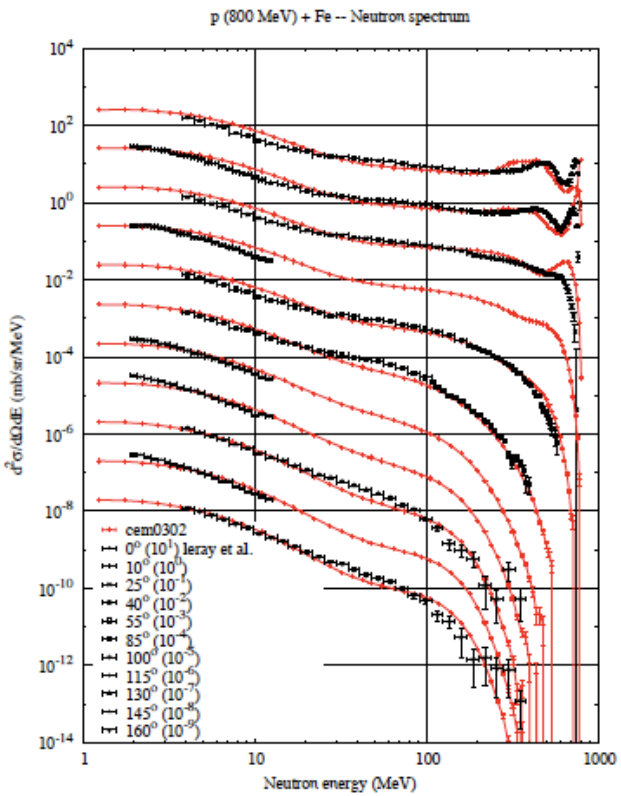
IAEA benchmark work on spallation models - 1

- Work started in Feb. 2008. Results: http://nds121.iaea.org/alberto/mediawiki-1.6.10/index.php/Main_Page

- INC models evaluated:
  - *CEM*03.02, CEM03.03
  - Cascade04, Cascade-ASF, Cascade-X
  - Geant4-Bertini, Geant4-BIC
  - *INCL4.5-ABLA07*, INCL4.5-Gemini, INCL4.5-SMM
  - ISABEL-ABLA07, ISABEL-Gemini, ISABEL-SMM
  - *MCNPX-Bertini*-Dresner
  - PHITS-Bertini, PHITS-jam, PHITS-JQMD

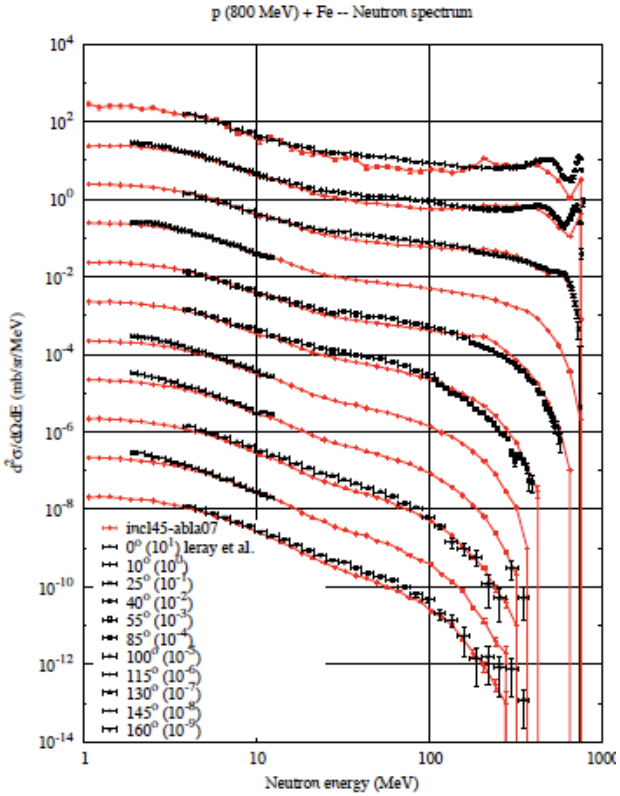
- Evaluation categories include:
  - Neutron production (double differential CS, multiplicity)
  - *Light charged particles* (H, D, T, S, A) double differential CS
  - Pion production, residue production, & excitation function

IAEA benchmark work on spallation models - 2, neutron production



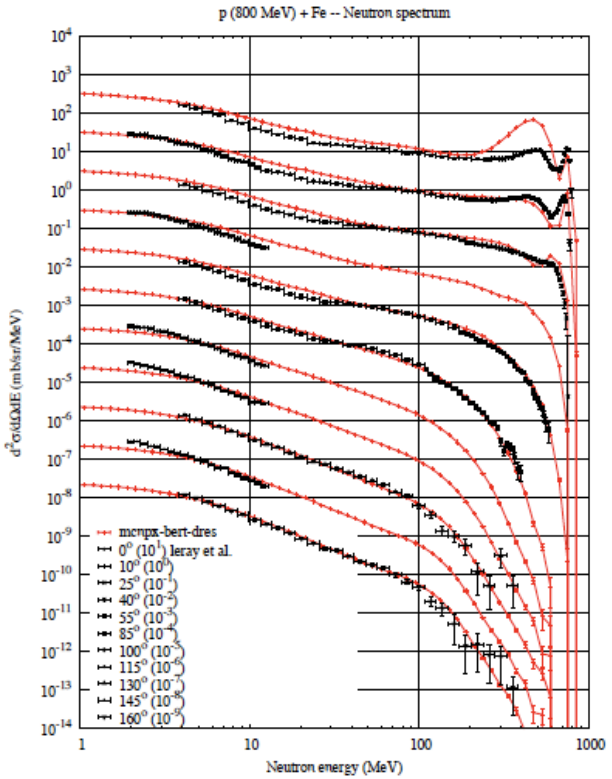
CEM03.02

S. Mashnik



INCL4.5-ABLA07

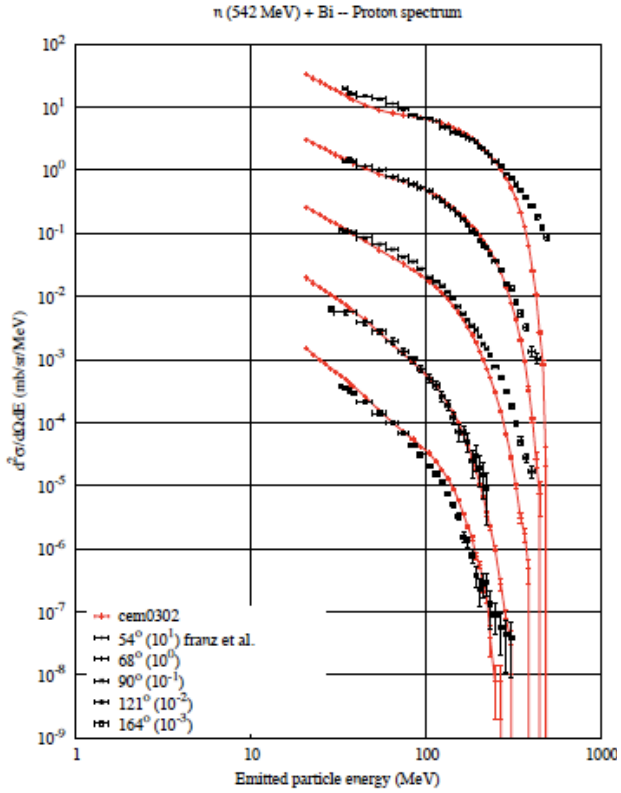
J. Cugnon, A. Boudard, A. Kelic, V. Ricciardi & D. Mancusi

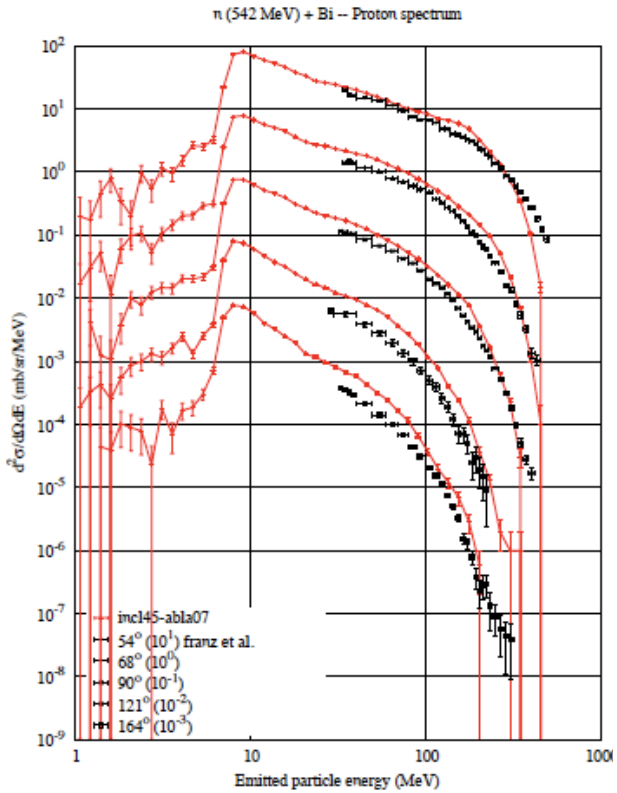


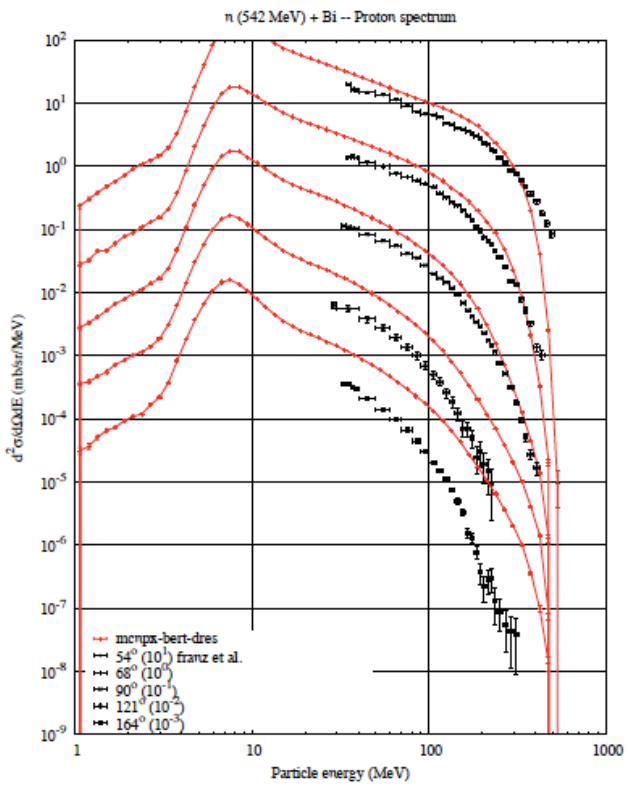
MCNPX-Bertini

F. Gallmeier & W. Lu

IAEA benchmark work on spallation models - 3, H production







CEM03.02

S. Mashnik

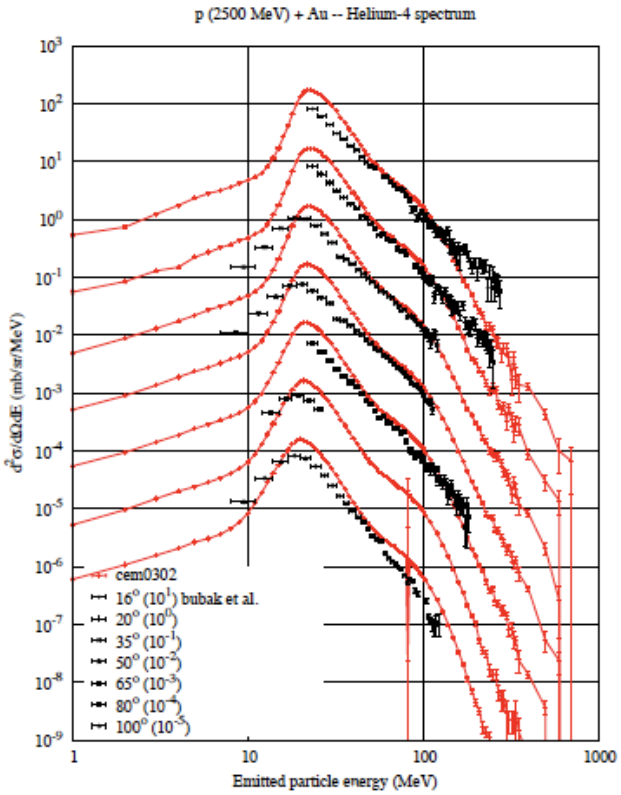
INCL4.5-ABLA07

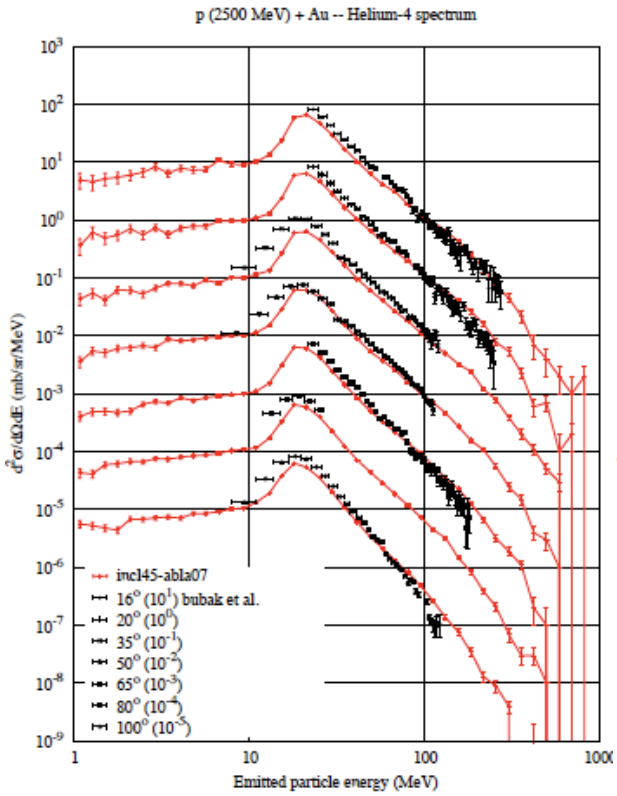
J. Cugnon, A. Boudard, A. Kelic, V. Ricciardi & D. Mancusi

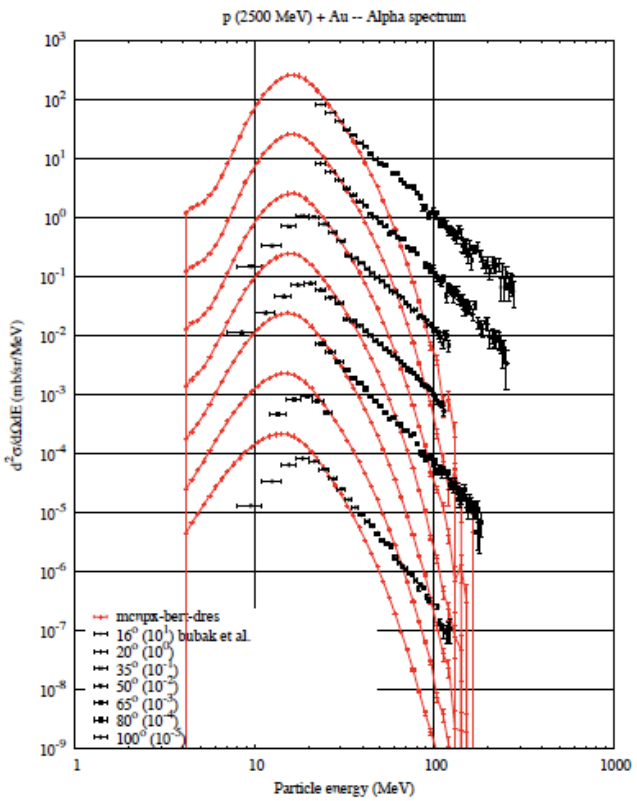
MCNPX-Bertini

F. Gallmeier & W. Lu

IAEA benchmark work on spallation models - 4, He-4 production







CEM03.02

S. Mashnik

INCL4.5-ABLA07

J. Cugnon, A. Boudard, A. Kelic, V. Ricciardi & D. Mancusi

MCNPX-Bertini

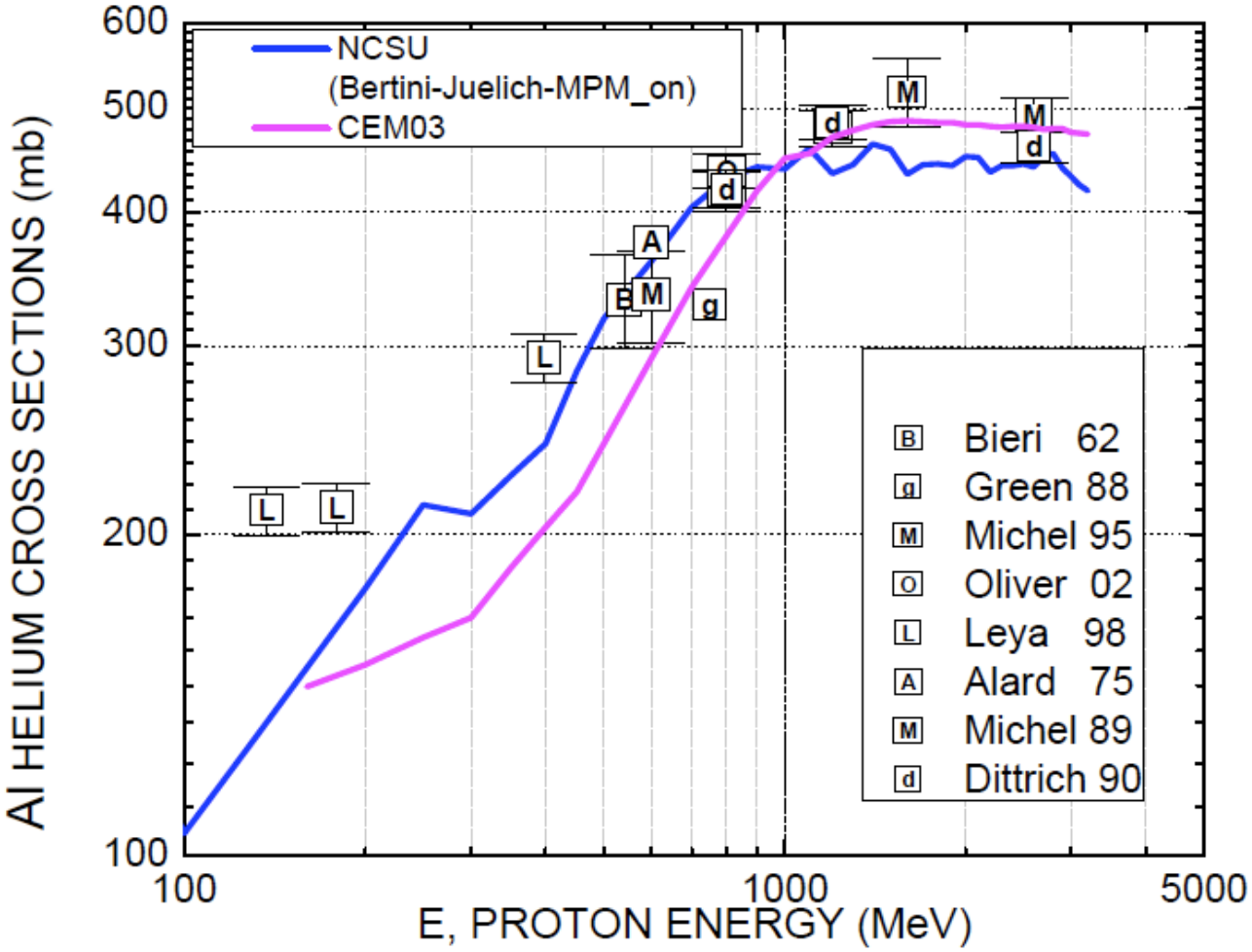
F. Gallmeier & W. Lu

IAEA benchmark work on spallation models - 5, General findings

- While most INC models perform well in describing the neutron production spectra
- For light charged particle emission [1]:
  - "7+ of the codes lack emission of composite particles in INC phase and are not able to describe the spectra at all"
  - "There is a trend that CASCADE-ASF and CEM03 codes perform best under 1 GeV incident and show weaknesses above"
  - "There is a trend that INCL4.5 codes perform weaker below 1GeV and improve above 1GeV"

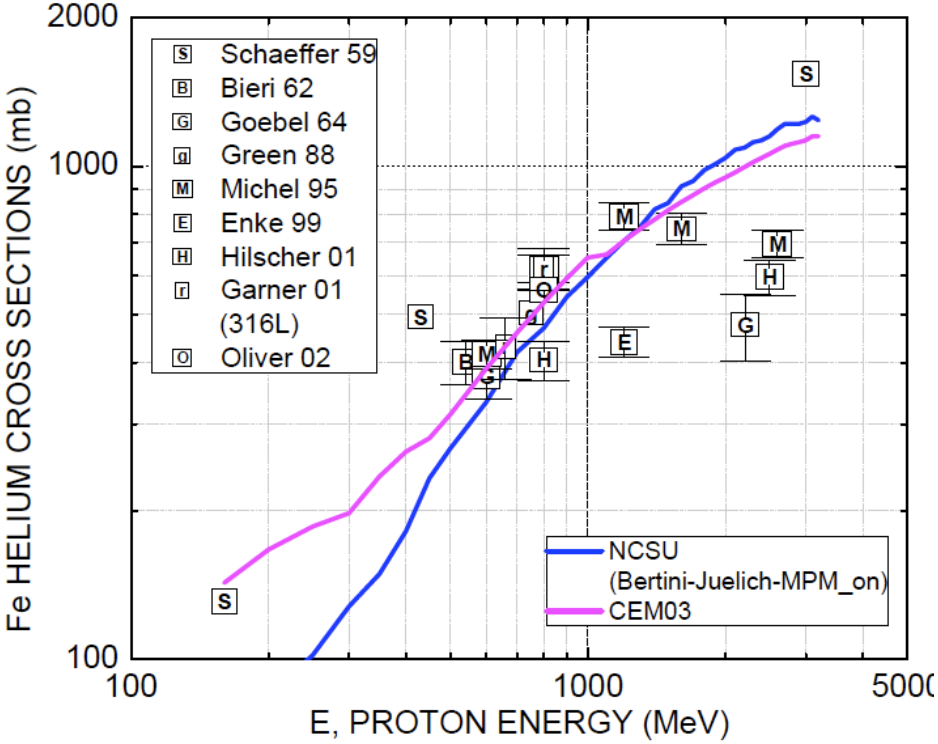
[1] F. Gallmeier, "The light charged particles benchmark evaluation", 2nd Advanced Workshop on Model Codes for Spallation Reactions, Saclay, France, Feb. 8-11, 2010

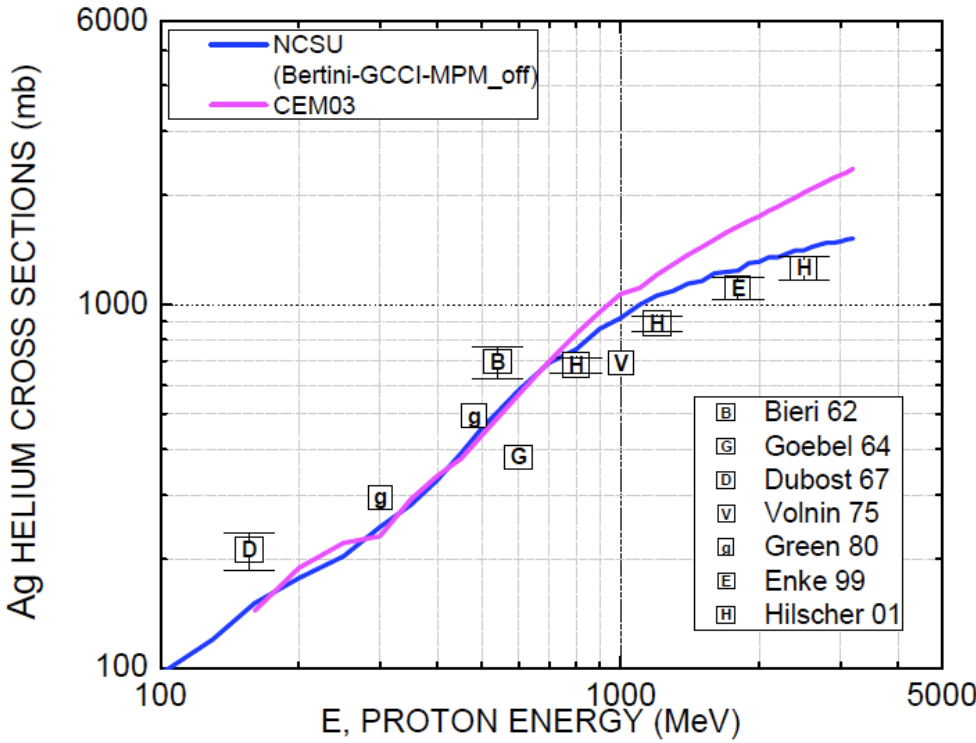
Results & discussion
- Helium cross section, 1



Al

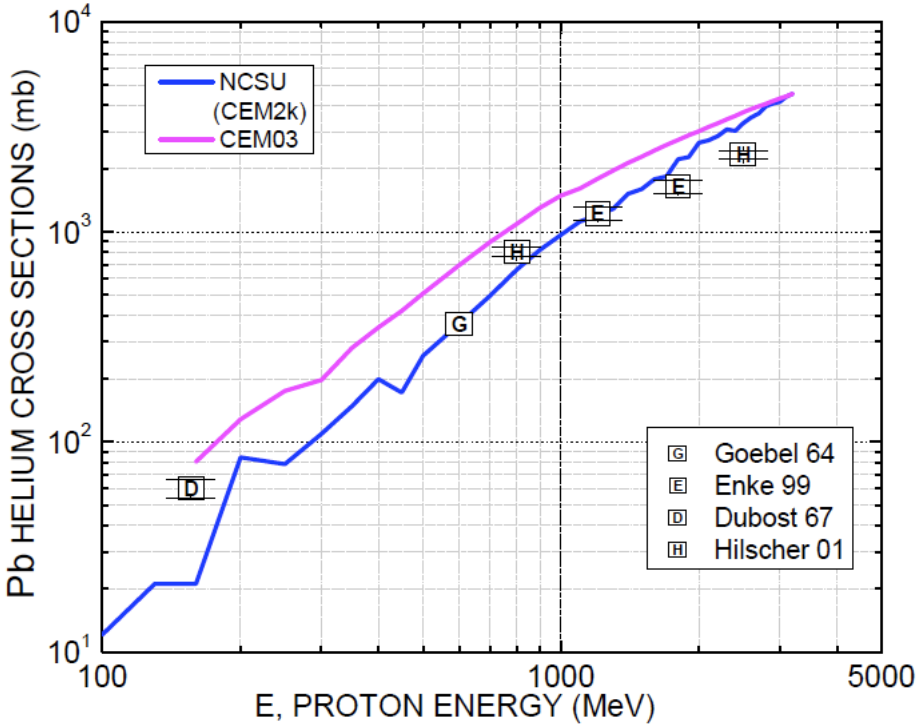
Results & discussion
- Helium cross section, 2

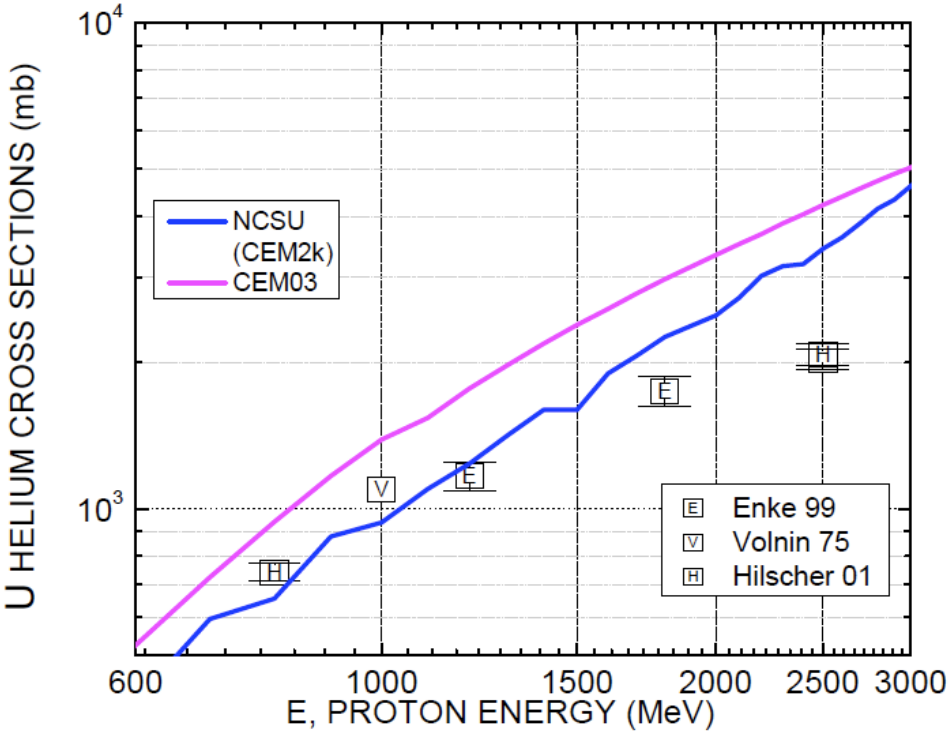




Fe ***Ag***

Results & discussion
- Helium cross section, 3



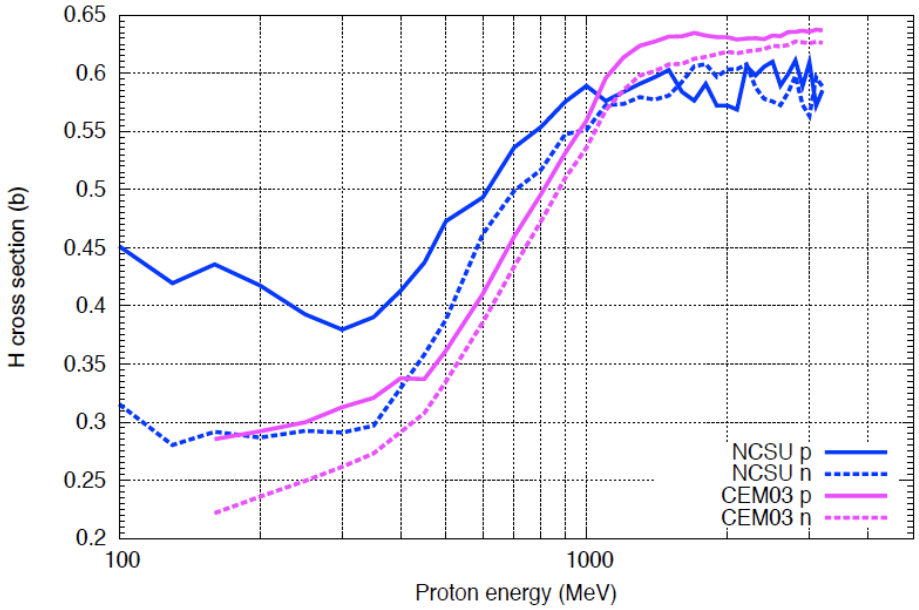


Pb ***U***

Results & discussion
- Helium cross section, summary

- For light targets, although slightly different from the Bertini results CEM03 calculated helium cross sections are in a reasonable agreement with the experiment data up to 3.2 GeV
- For intermediate-weighted and heavy targets, CEM03 performs well for energies below 1 GeV but not better than NCSU results for energies above 1 GeV

Results & discussion
- Hydrogen cross section, 1



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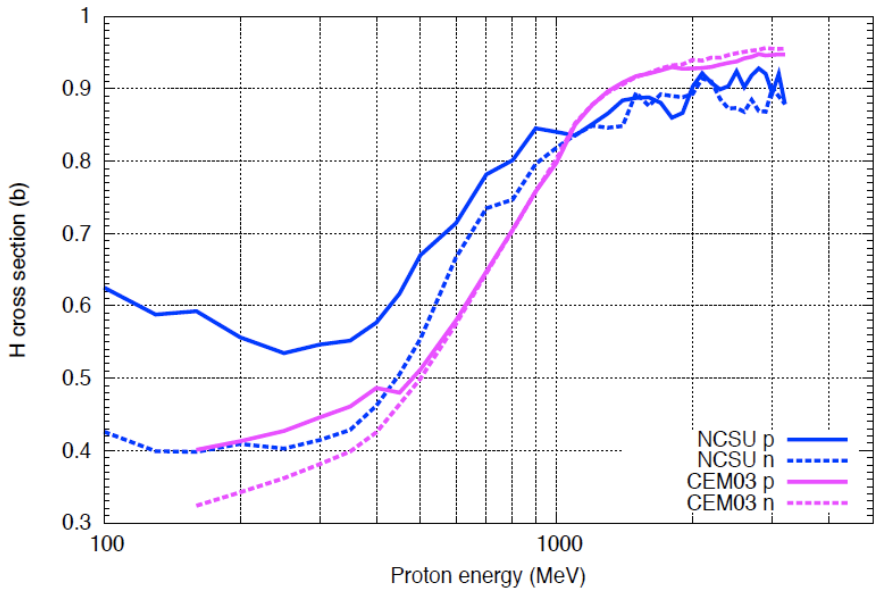
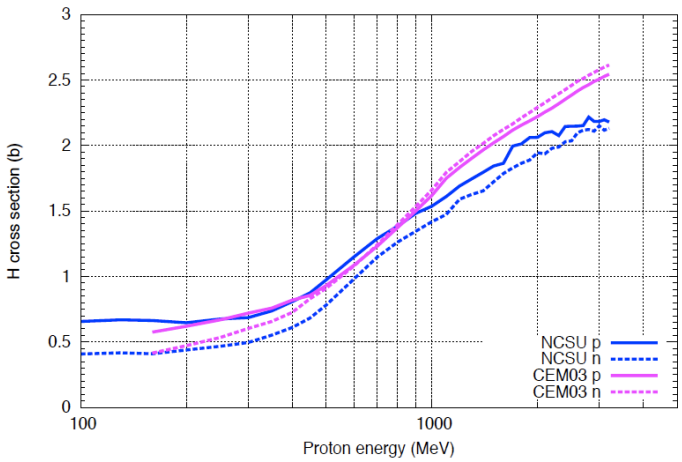


Si

Results & discussion
- Hydrogen cross section, 2



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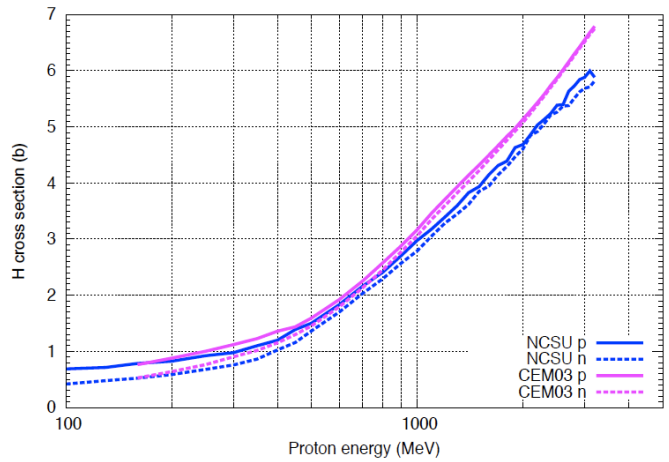

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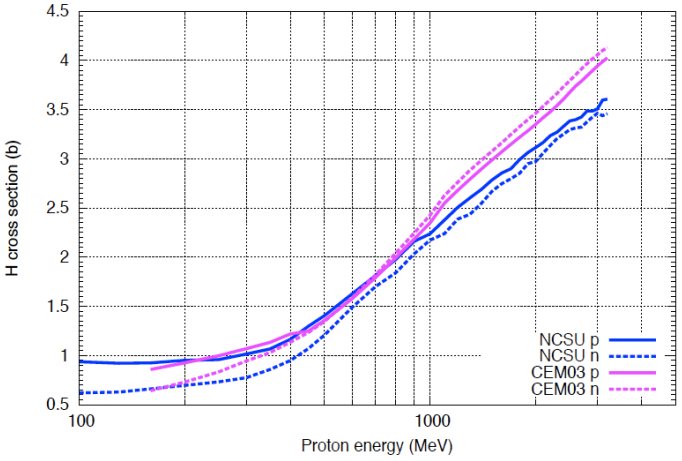

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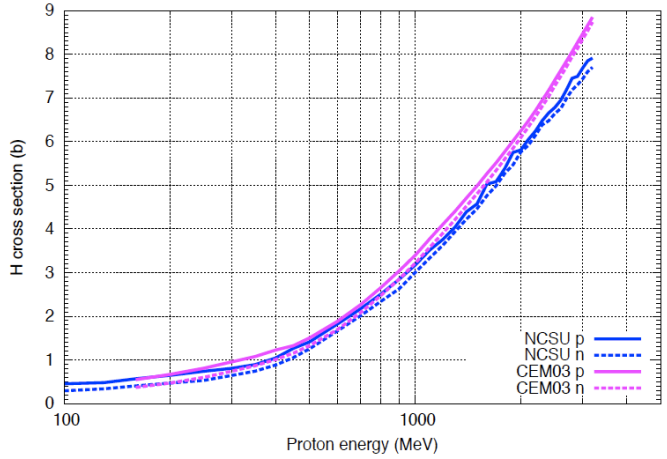
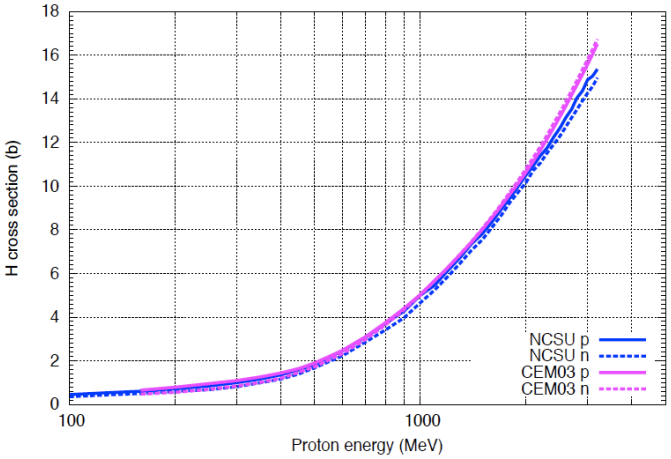


Sn

Results & discussion
- Hydrogen cross section, 3



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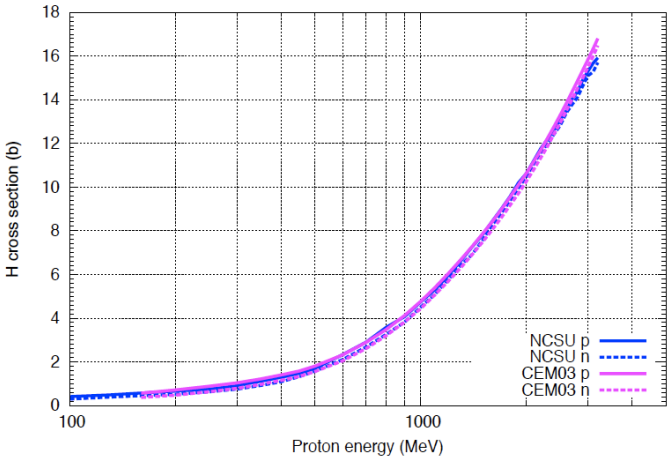

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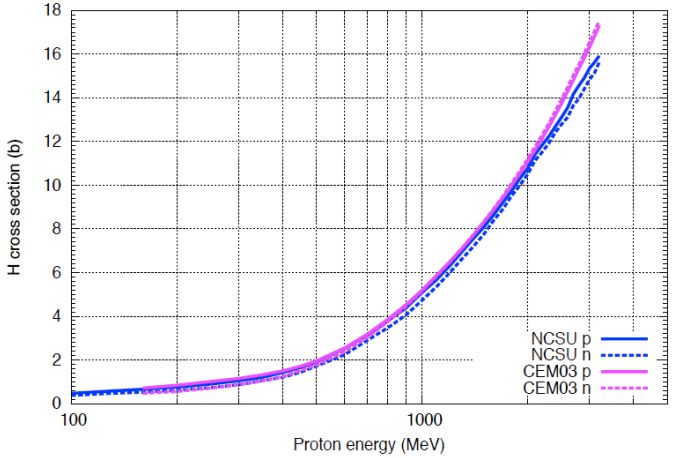

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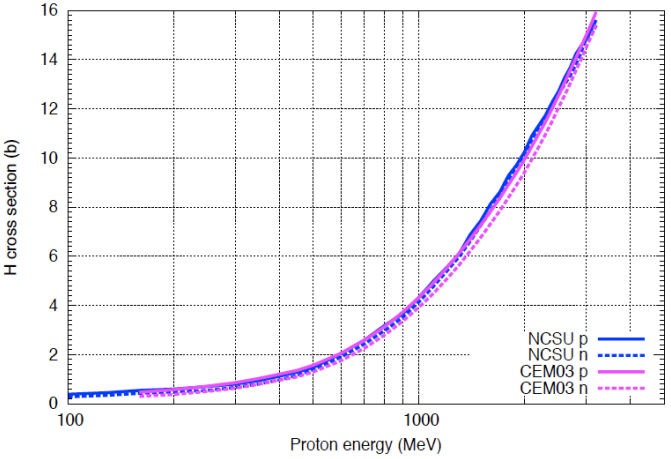
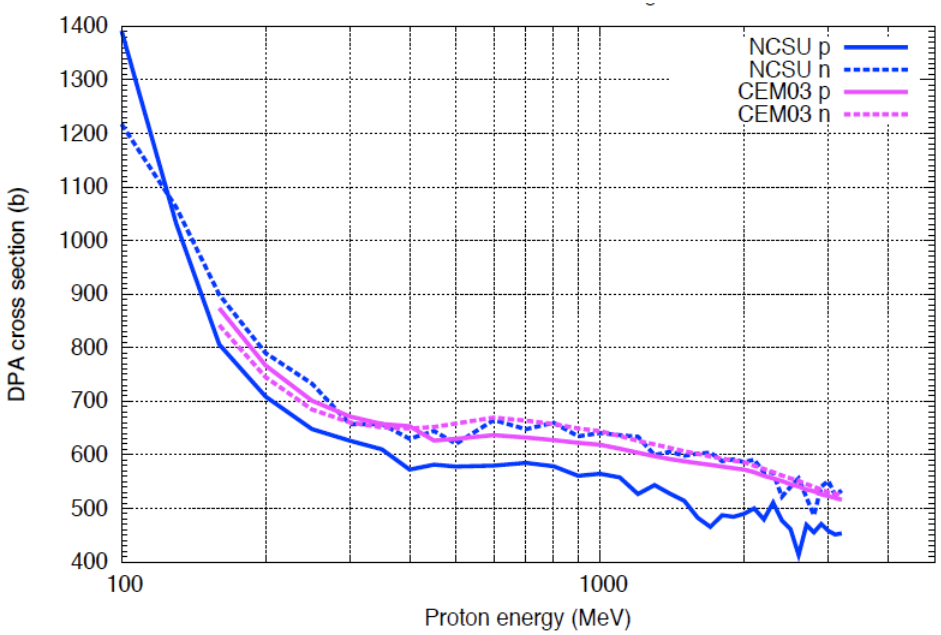


Pb

Results & discussion
- Hydrogen cross section, summary

- For light targets, CEM03 results show > 30% difference with the Bertini calculated cross sections in the NCSU database at ~ 200 MeV. The difference is reduced to ~10% for energies above 1 GeV.
- For intermediate-weighted and heavy targets, CEM03 results generally agree well with the Bertini calculated cross sections.
- As targets get heavier, CEM03 results become more and more close to the Bertinit calculated cross sections. For Z>79, CEM03 results are almost identical to those from Bertini.

Results & discussion
- Displacement cross section, 1



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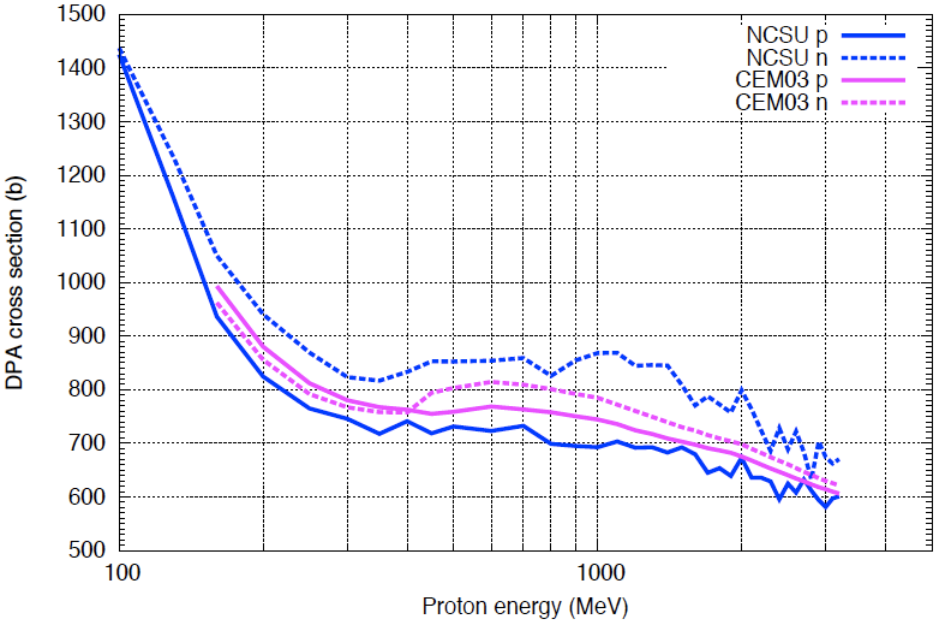

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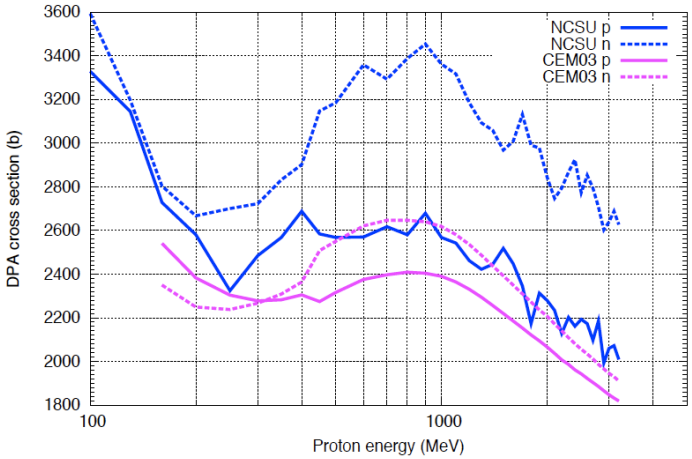
Results & discussion
- Displacement cross section, 2



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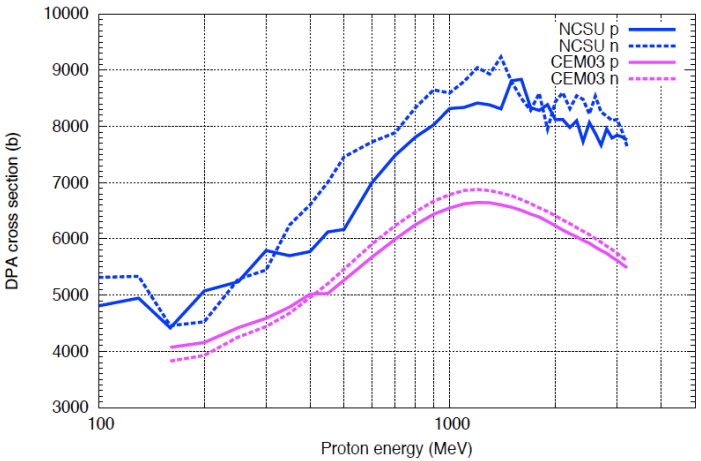

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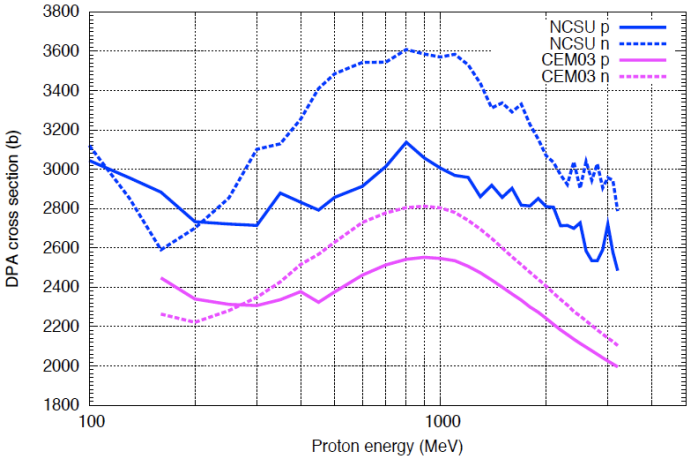

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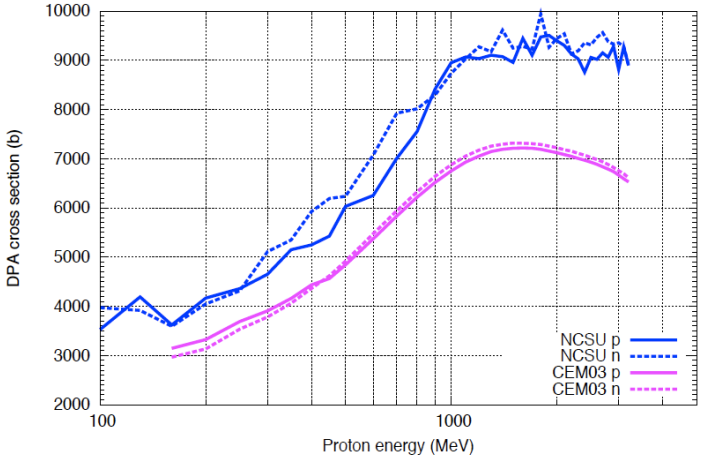
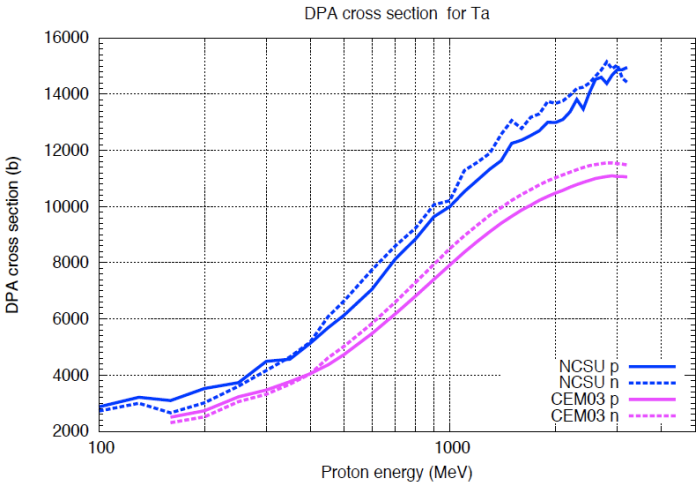


Sn

Results & discussion
- Displacement cross section, 3



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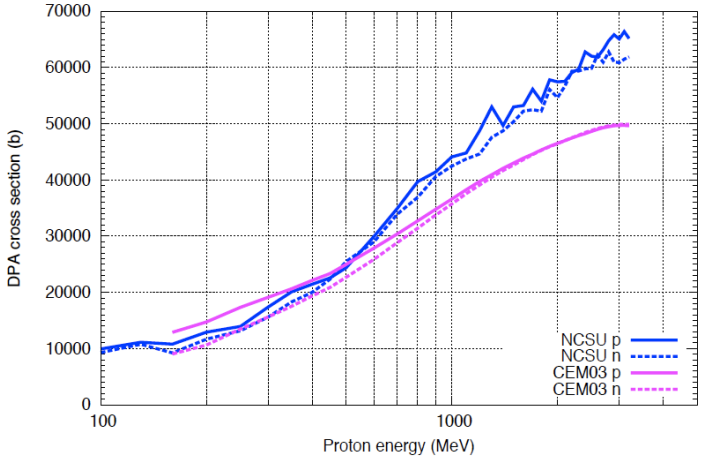

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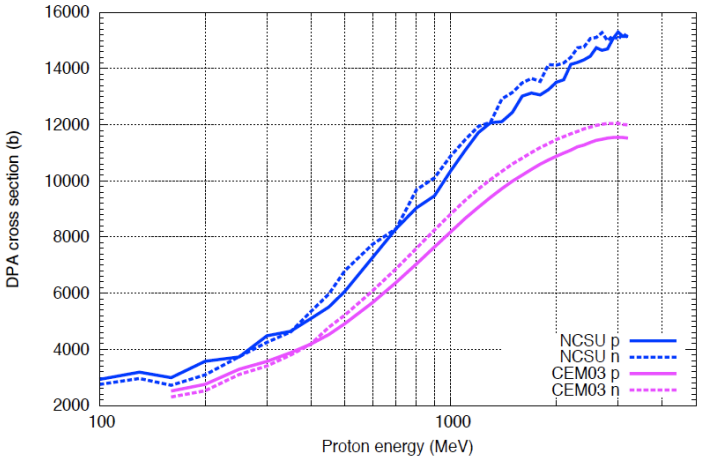

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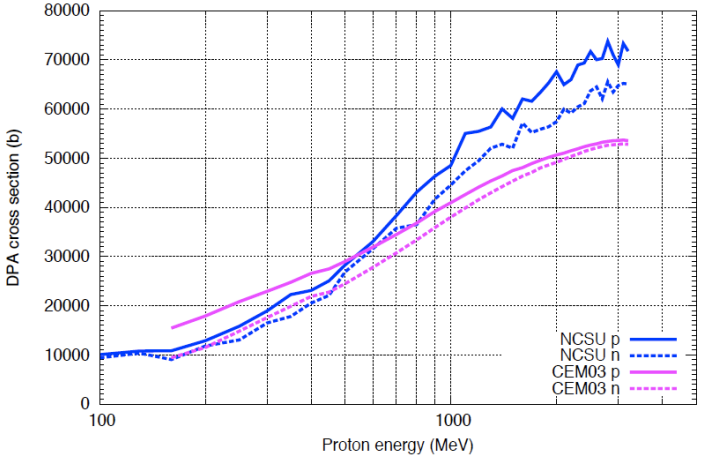
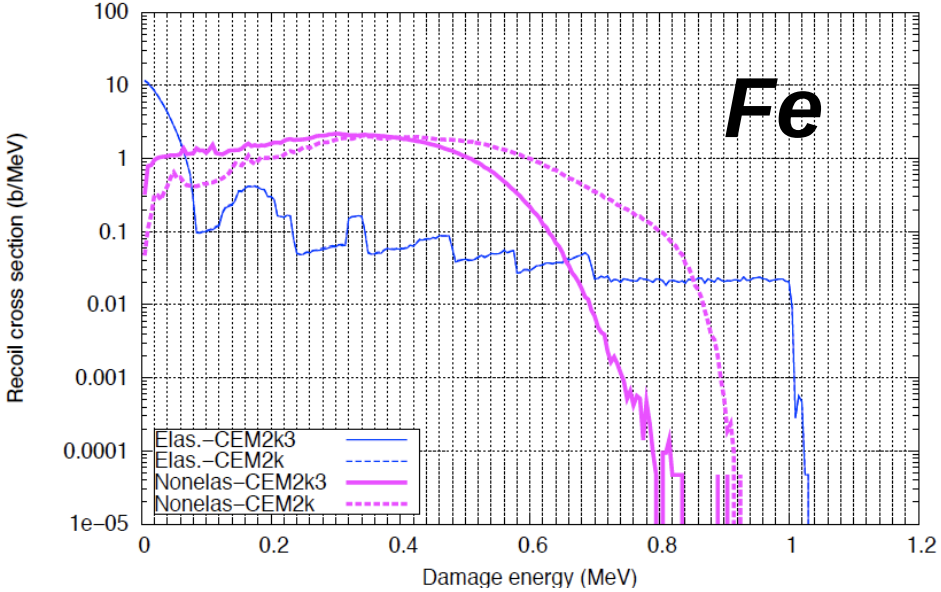


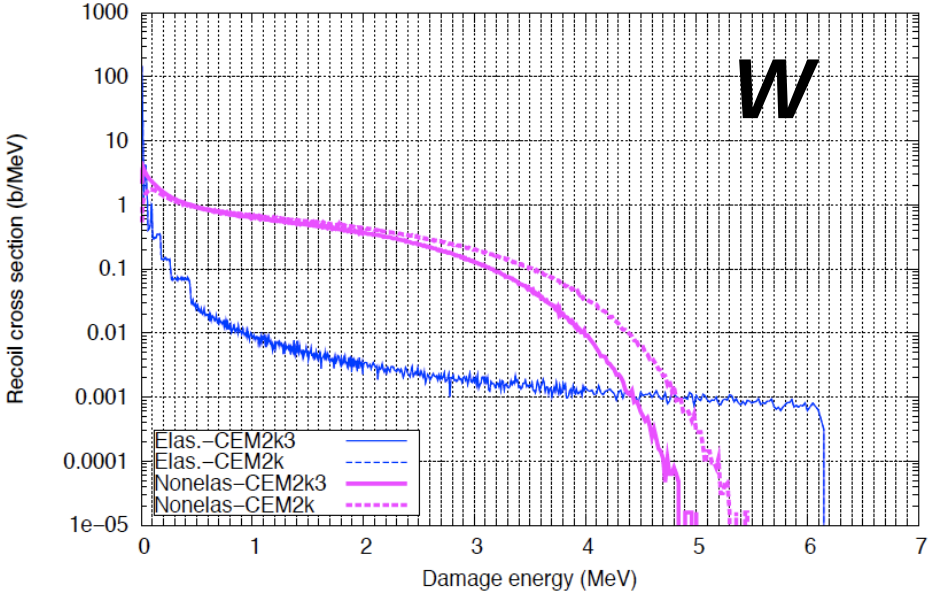
Pb

Results & discussion
- Displacement cross section, summary

- For light targets, CEM03 results agree reasonable well with the CEM2k calculated cross sections in the NCSU database. The difference is < 10%.
- For intermediate-weighted targets with Z<30, CEM03 results show constantly ~20% reduction for proton induced displacement cross sections and ~30% for neutron induced displacement cross sections compared to the CEM2k results.
- As targets with Z>30, CEM03 results are ~10% lower than CEM2k results at ~200 MeV. The gap is widened as incident energy increases and reaches ~30% at ~3 GeV.

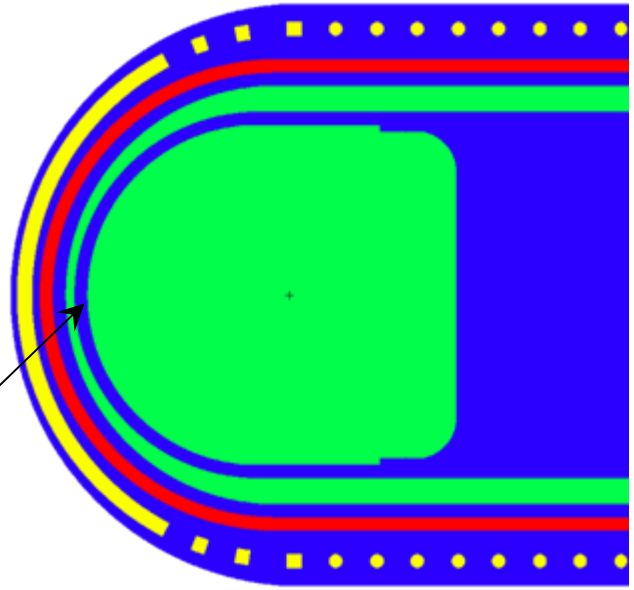
Results & discussion - Displacement C.S. , possible explanation





- The PKA spectra shown here are the bombing results of 1000 MeV neutrons
- Compared to CEM2k, the results from CEM03 show less high energy recoils and more low high energy recoils.
- Correspondingly, CEM03 shortens the pre-equilibrium stage and extends the evaporation stage

Radiation damage on SNS target vessel



	Displacement (DPA)		Helium (appm/yr)		Hydrogen (appm/yr)	
	NCSU	CEM03	NCSU	CEM03	NCSU	CEM03
N induc.	11.5	11.5	131	149	929	880
P induc.	9.6	8.3	1746	1984	7375	6942
Total	21.1	19.9	1877	2133	8305	7823

Summary

- CEM03 is used to recalculate the displacement, He & H cross sections previously evaluated in the NCSU radiation damage database for energies > 150 MeV
  - CEM03 shows improvement in the helium cross section at energies below 1 GeV, still not good above 1 GeV
  - CEM03 calculated hydrogen cross sections show a surprising trend of agreement with the Bertinit results
  - In a rebalance of pre-equilibrium stage and evaporation stage to favor the emission of light charged particles, CEM03 shows a 20-30% reduction in the displacement cross section
- For He & H cross sections, NCSU radiation damage database stands well even though INC models have gone through major revision and improvement.
- For displacement cross sections, NCSU radiation damage database needs to be reevaluated at least for the sake of the statistical error.

Future work

- Further investigation of the reduction in the displacement cross section calculated by CEM03
- Use most recent INCL version to calculate He & H cross sections at energies above 1 GeV