# Status of Neutron High Precision Models

Koi, Tatsumi

SLAC National Accelerator Laboratory

# Outline

- G4NDL
- Neutron High Precision (HP) model and cross section
- G4NeutronHPThermalScattering
- Update of format

# G4NDL

- The neutron data files for High Precision Neutron models
  - Based on ENDF files
- Until v3.7 maintained by H. P. Wellisch
  - Without information of parent ENDF files
- Since v3.8 (v3.14 is the latest)
  - Add nucleus on demand with information of parent files
  - Fix errors
- The data format is similar ENDF-6, however it is not equal to.
  - Many entries are only existed in ENDF files but not in G4NDL.
- Resonance reconstructions are processed by “NJOY” (recon)
- 0 K data
  - Doppler broadening calculated for every cross section request

# Neutron High Precision (HP) model and cross section

- Low energy (<20MeV) neutron transportation model
  - Data (G4NDL) driven model
- 4 models and cross sections
  - Elastic(In reaction nomenclature of ENDF: MT2)
  - Inelastic
  - Capture(MT102)
  - Fission(MT18) model and cross section
  - Inelastic = MT1 – MT2 – MT 102 – MT18
- Not all the ENDF-6 Format supported
  - "Format" means how the data are arranged in the libraries and give the formulas needed to reconstruct physical quantities such as cross sections and angular distributions from the parameters in the library
  - Recent released libraries (ENDF-VII and so on) are used "Format" those were not employed before.
  - This is the main reason we do not fully update to ENDF-VII or later libraries

# “G4NEUTRONHP_NEGLECT_DOPPLER”

- NeutronHP uses 0K data and apply effects of thermal motion of target nuclei on the fly.
- However this requires CPU cost a lot.
  - Especially in high tempareture.
- If user set the environment variable of “G4NEUTRONHP_NEGLECT_DOPPLER”, the effects will be neglect in the calculation of cross section.
  - The effects still take into account in final state calculation
- In most case, getting reasonable result with much faster(x5) calculation speed.
  - Some validation plot will be provided in this presentation
- However an essential solution is using the G4NDL data which reconstruct at the temperature of interested.
  - Need design change!

# Energy and momentum conservation in NeutronHP

- NeutronHP is a data driven model and not designed for the conservation at single interaction level.
- However there were many space for improvements
  - Breaks in two body interaction
  - Break of baryon number conservation
    - Residual missing
- Now we apply tunings in final states for better physics performance.
  - Still not perfect
  - You can skip this tuning by setting the environment variable of "G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE"

# Impact of the tuning introduced at v9.2

**9.1.p01**

| Reaction | Number of event | Momentum | Energy | Charge | Baryon |
|---|---|---|---|---|---|
| (n,n*) | 355 | 1 | 0 | 0 | 0 |
| (n,2n) | 1521 | 1 | 1 | 1 | 1 |
| (n,na) | 6 | 1 | 1 | 1 | 1 |
| (n,np) | 42 | 1 | 1 | 1 | 1 |
| (n,p) | 59 | 1 | 0 | 0 | 0 |
| (n,d) | 20 | 1 | 0 | 0 | 0 |
| (n,t) | 2 | 1 | 0 | 0 | 0 |
| (n,a) | 14 | 1 | 0 | 0 | 0 |

**9.2**

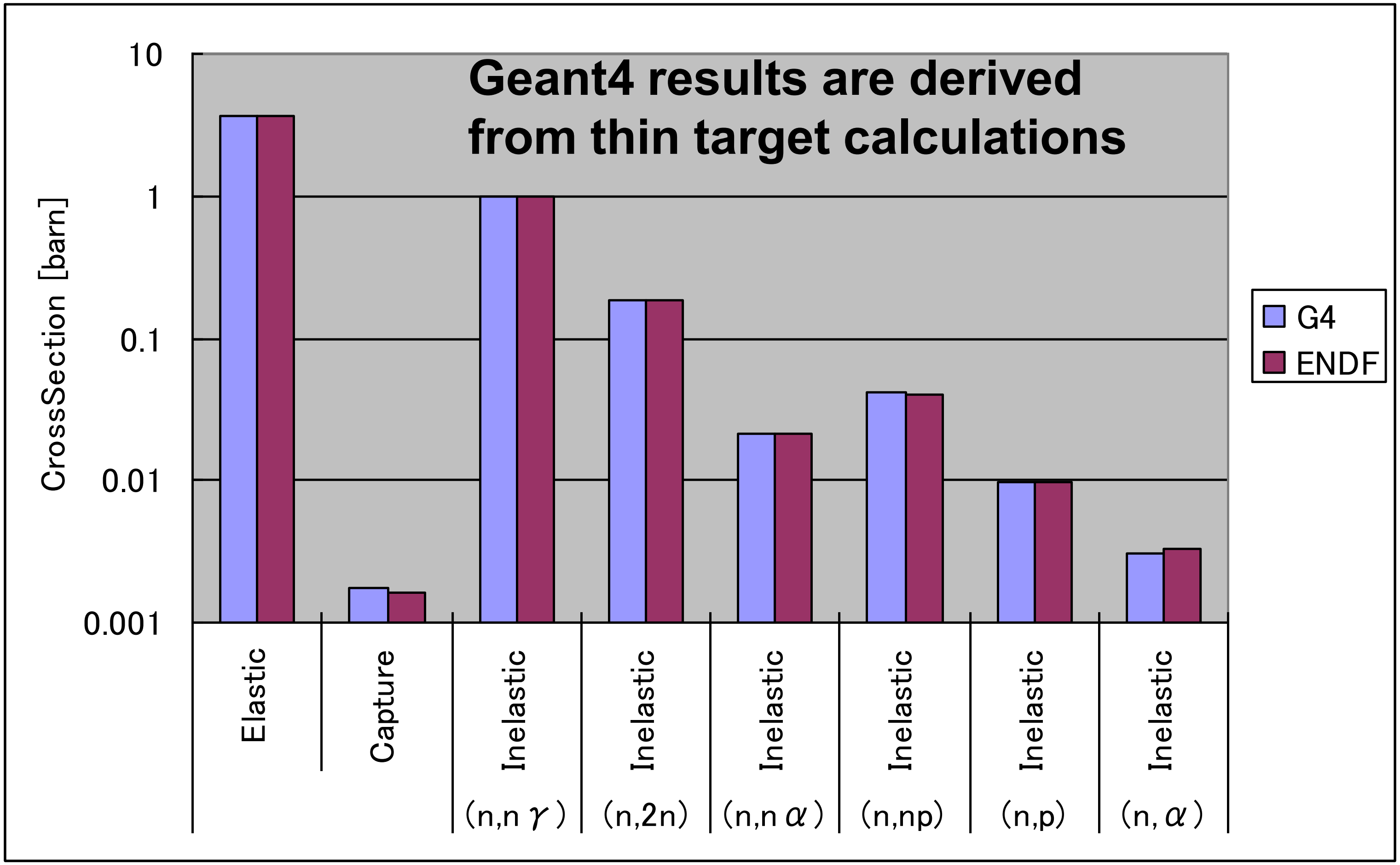
| Reaction | Number of event | Momentum | Energy | Charge | Baryon |
|---|---|---|---|---|---|
| (n,n*) | 385 | 0 | 0 | 0 | 0 |
| (n,2n) | 1519 | 0 | 0 | 0 | 0 |
| (n,na) | 7 | 0 | 0 | 0 | 0 |
| (n,np) | 33 | 0 | 0 | 0 | 0 |
| (n,p) | 38 | 0 | 0 | 0 | 0 |
| (n,d) | 12 | 0 | 0 | 0 | 0 |
| (n,t) | 5 | 0 | 0 | 0 | 0 |
| (n,a) | 22 | 0 | 0 | 0 | 0 |

18 MeV neutron hit of 72Germanium

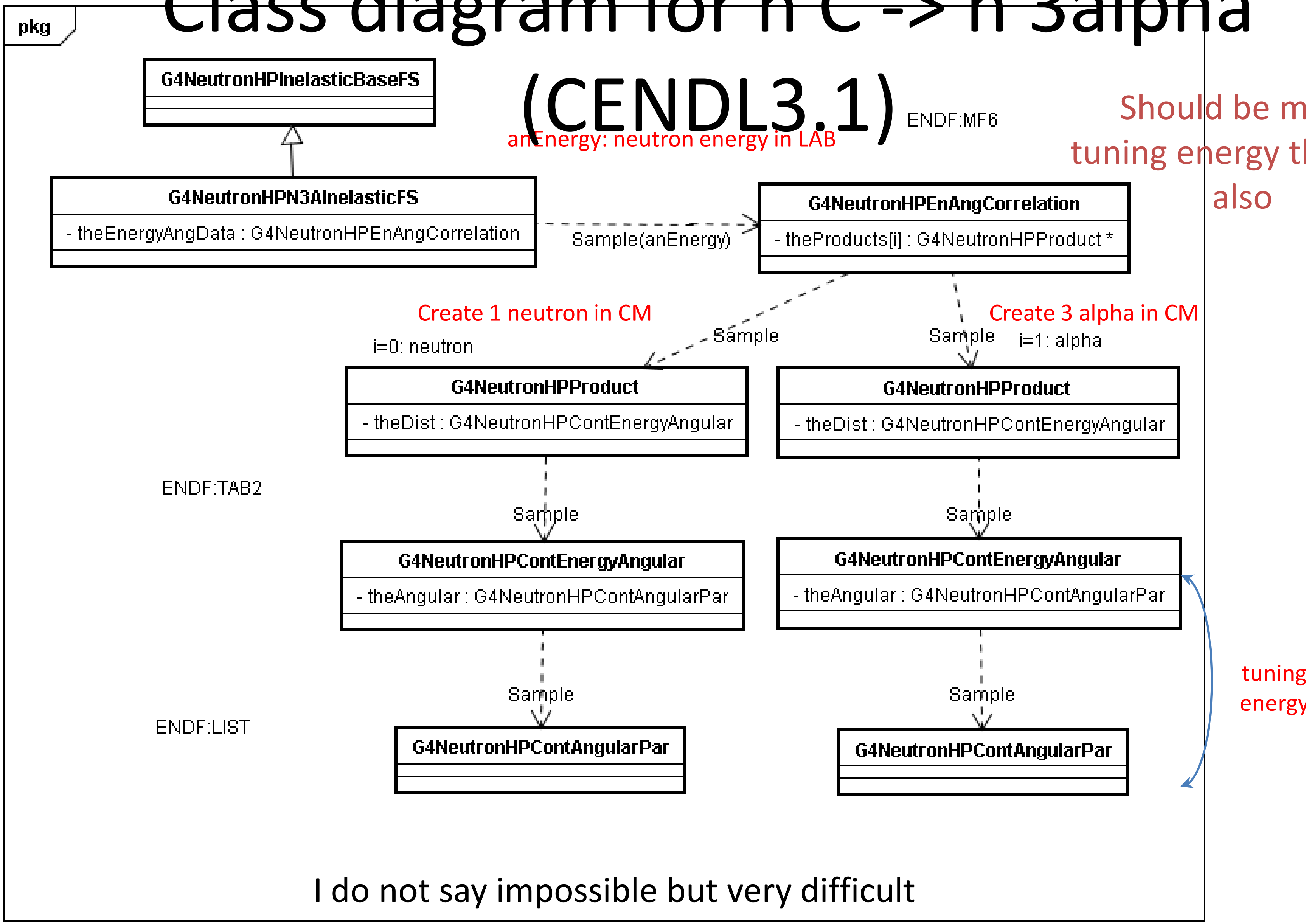
Event fail: abs(PorEbefore/PorEafter) >1.0e-5

# Verification of High Precision Neutron models Channel Cross Sections

## 20MeV neutron on $^{157}$Gd



# Typical neutron HP reaction Class diagram for n C -> n 3alpha (CENDL3.1)



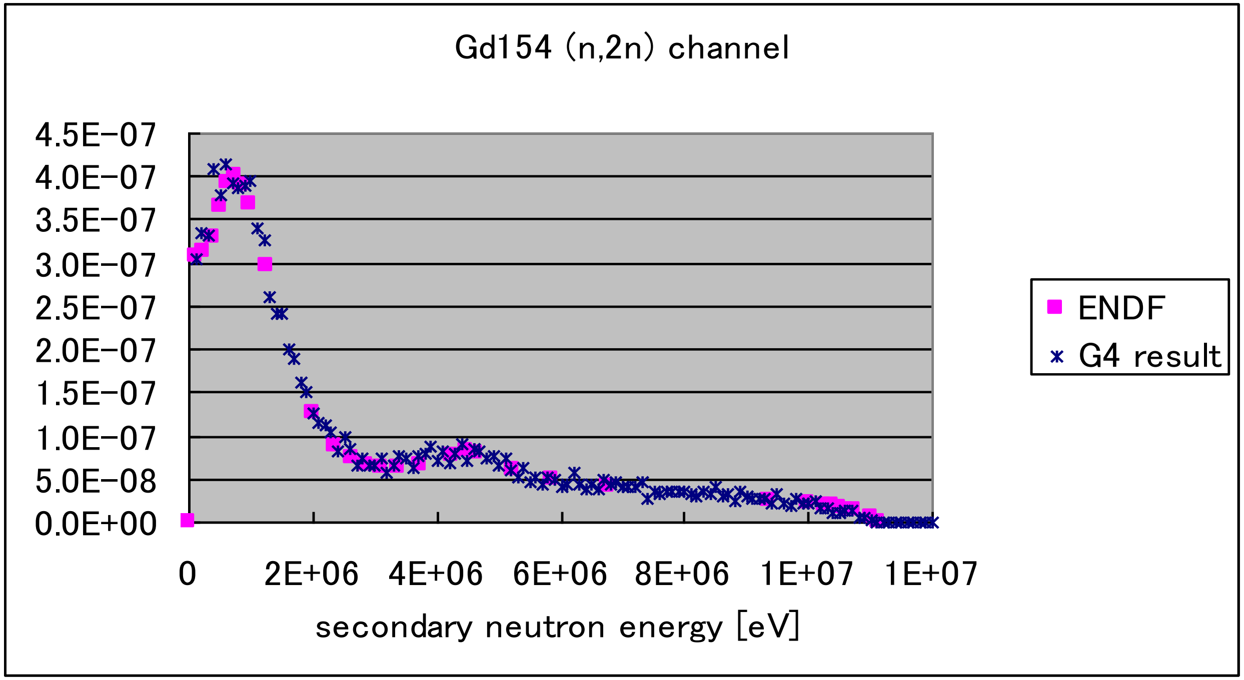

Should be made tuning energy this level also

I do not say impossible but very difficult

# Be9(n,2n)Be8

- Final state of this reaction is described in MF6
- 2 particle distributions given in the laboratory frame
  - LAW=7 (Laboratory Angle-Energy Law) is used
- NeutronHP expected 2 particle means neutrons and Be8
- However the evaluation (ENDF-VI, I believe), it returns neutrons and alphas
  - Decay of Be8 is not always included
    - Sometime Be8 also exists in Final state
- As the result, unexpected high energy photons are produced in the reaction.
- Artificial hack is applied at v9.4
  - However I am not sure that this hack is effective or valids in other evaluations.

# Verification of High Precision Neutron models
# Energy Spectrum of Secondary Particles



# ATLAS Cavern Background Simulation

- Physics List
  - QGSP_BERT
  - QGSP_BERT_HP
  - QGSP_BERT_HP with option "G4NEUTRONHP_NEGLECT_DOPPLER"
- Geometry "Atlas Cavern Background Simulation"

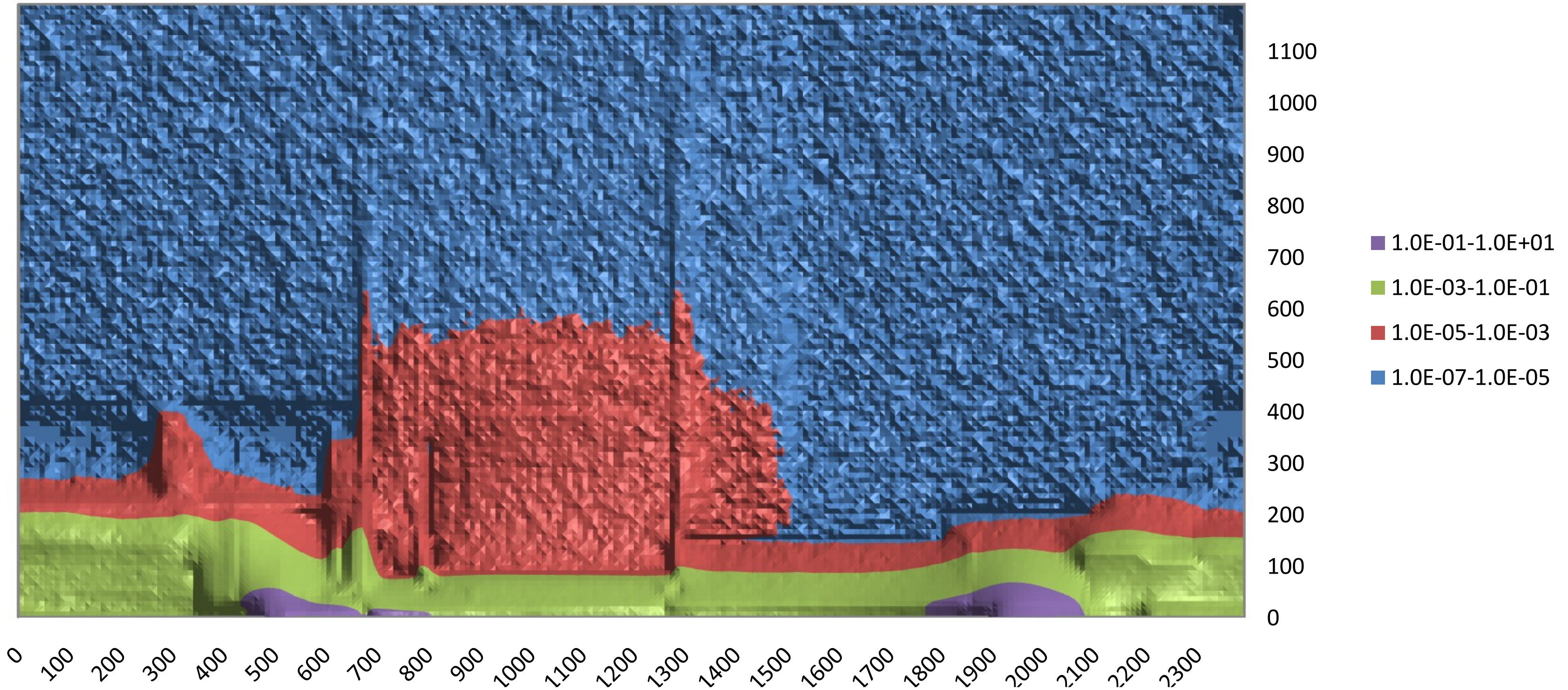
# Comparison of CPU and Memory Consumption

based on ATLAS Cavern Background 64 7TeV pp events

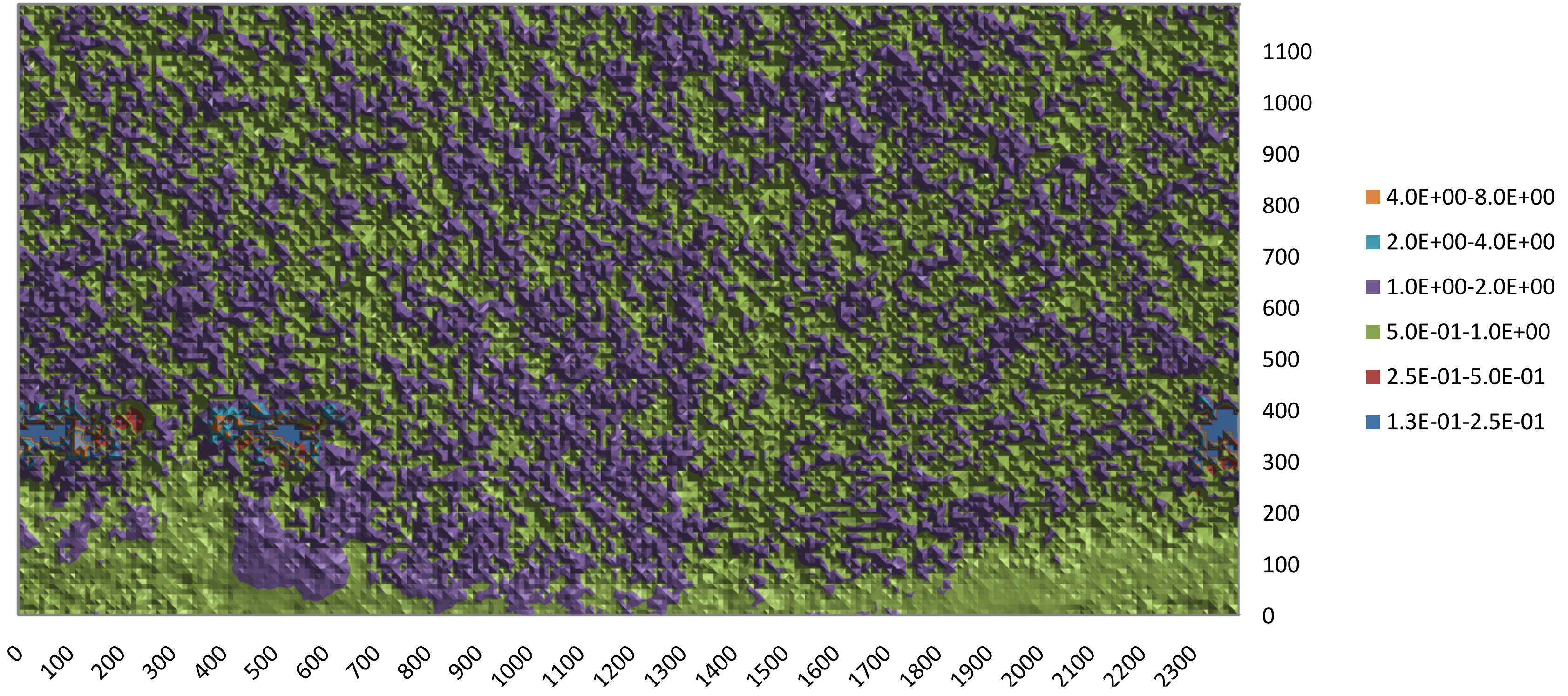
- QGSP_BERT
  - 180 sec/event, 125MB
- QGSP_BERT_HP (FULL)
  - 1,200 sec/event, 690MB (values from 16 events)
- QGSP_BERT_HP (Neglect Doppler Broadening)
  - 280 sec/event, 710MB

# QGSP_BERT_HP
# neutorn

neutrons per cm$^2$ per pp event



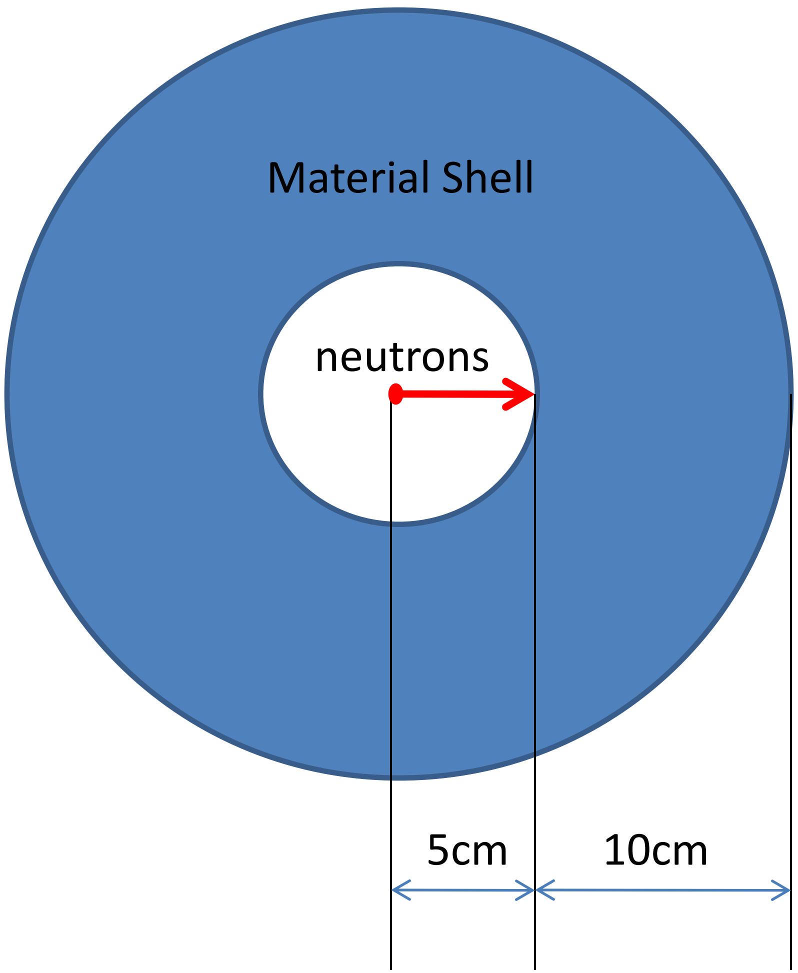
# QGSP_BERT_HP/QGSP_BERT_HP(ND)
# neutorn



# GAMOS comparison

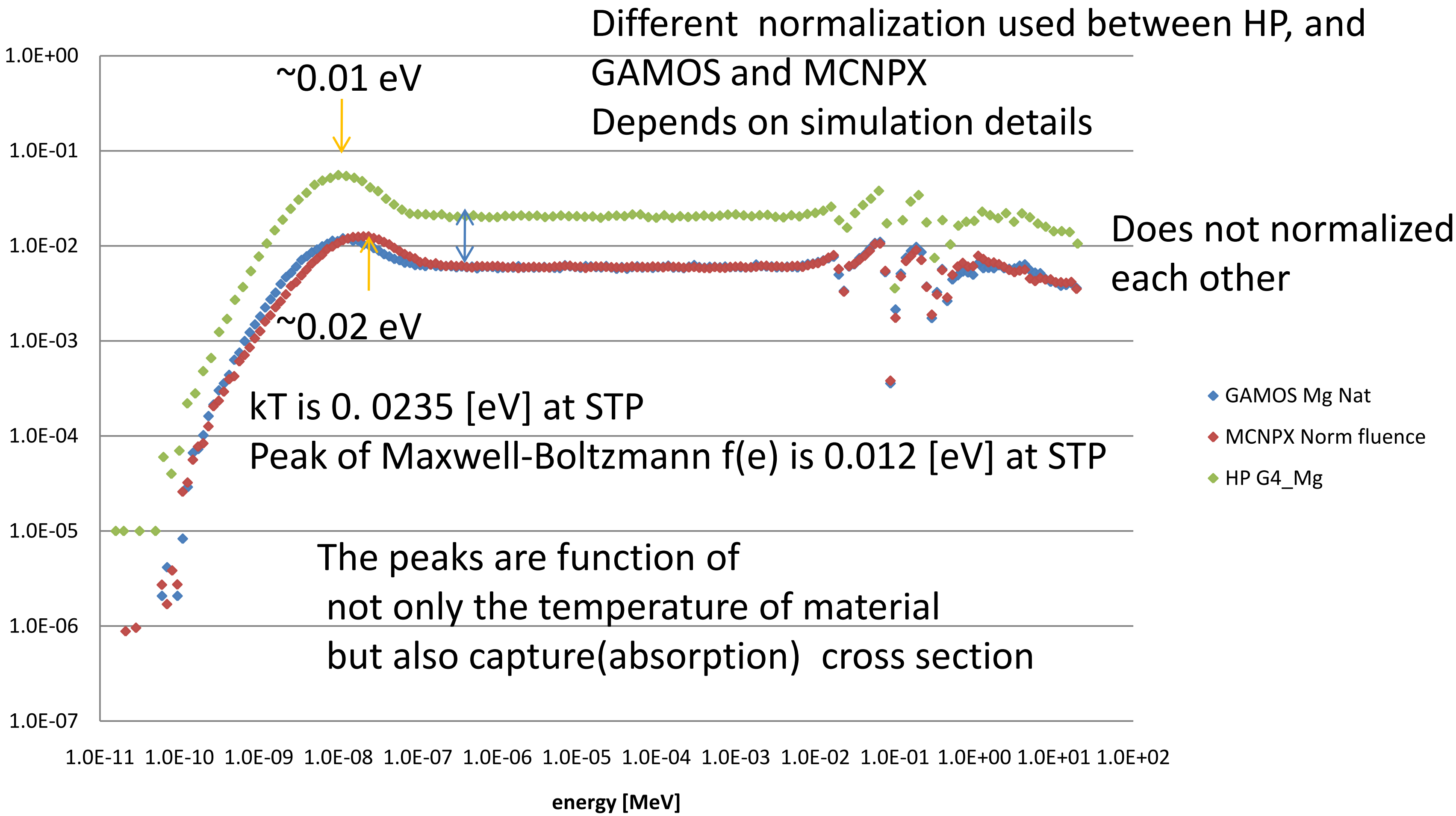
- Requested by Pedro
- Neutron energy spectrum after certain amount (10cm) of materials
  - O16 O17 Na23 Mg Nat Al1327 Si28 Si29 Si30 Cl1735 Cl1737 K nat Ca nat Fe 54 fe56 Fe57 Fe58 Mn55 Pb204 Pb206 Pb207 and Pb208
- His main interested is shape and position of thermal peak.
  - In some case there are relatively large deference to MCNP result

# Condition of GAMOS comparison



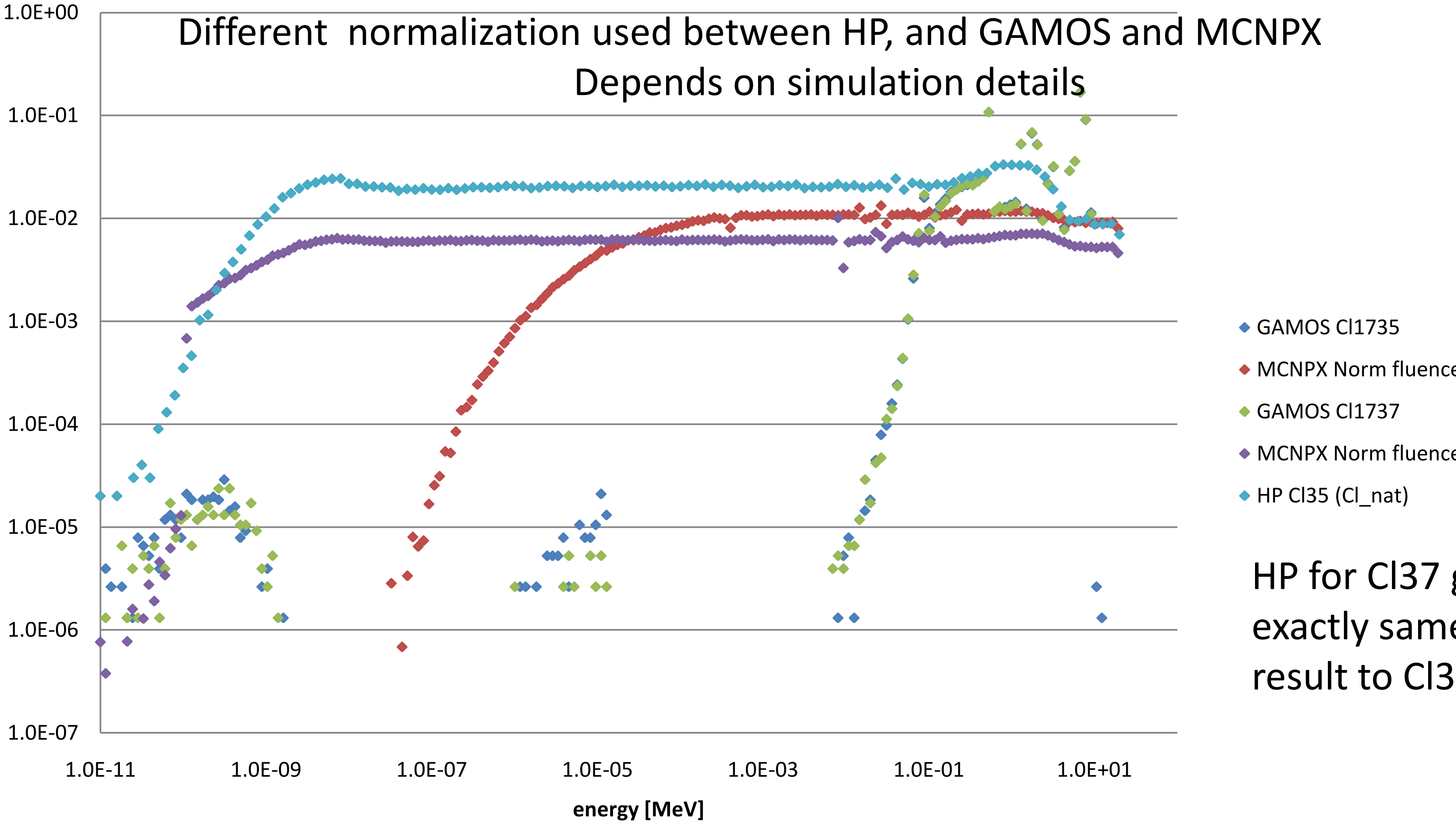

- Neutron from the center of the sphere.
- Energy of source neutron
  - flat in the logarithm of the energy, from 1E-11 to 19 MeV
- Material shell has thickness of 10cm
- Measure energy of neutrons at the outer surface of the shell

# Magnesium



Different normalization used between HP, and GAMOS and MCNPX
Depends on simulation details
~0.01 eV
~0.02 eV
Does not normalized each other
kT is 0. 0235 [eV] at STP
Peak of Maxwell-Boltzmann f(e) is 0.012 [eV] at STP
The peaks are function of
not only the temperature of material
but also capture(absorption) cross section
1.0E+00
1.0E-01
1.0E-02
1.0E-03
1.0E-04
1.0E-05
1.0E-06
1.0E-07
1.0E-11 1.0E-10 1.0E-09 1.0E-08 1.0E-07 1.0E-06 1.0E-05 1.0E-04 1.0E-03 1.0E-02 1.0E-01 1.0E+00 1.0E+01 1.0E+02
energy [MeV]
GAMOS Mg Nat
MCNPX Norm fluence
HP G4_Mg

# Cl35 and Cl37




HP for Cl37 gives exactly same result to Cl35

# General status of validation

- Cross sections (Elastic, Inelastic, Capture and Fission)
  - Well validated except for resonance structures (and thermal peak(?))
- Final states
  - Elastic
    - Reasonably validated
  - Inelastic
    - Better than before, but many gaps in energy distribution of secondary particles
  - Capture
    - Better than before, but many gaps in energy distribution and multiplicities of secondary photons
  - Fission
    - No systematic validation at all
    - When I succeeded the package, I fixed all the trivial but lethal (make core dump) bugs.

# A few comments for ENDF

- "The ENDF system was developed for the storage and retrieval of evaluated nuclear data to be used for applications of nuclear technology" from "Philosophy of the ENDF System in ENDF-6 Formats Manual
  - Detailed care for secondary neutrons
- Evaluation are done with not only experimental data but also theoretical calculations
- Do not provide full set of required information
  - Sometime (many time) only channel cross sections are given
  - The same reaction is described in several FORMAT among the evaluations (ENDF, JENDL, JEFF, CENDL and so on).

# Issues for G4NDL and NeutronHP

- Checking completeness of supported FORMAT
  - All FORMAT which are used in the recent libraries (ENDF-VII, JEND4.0, JEF3.1 and so on) is supported or not?
- Re-design both data format and package classes
  - Data Format
    - Enable to use temperature specified data
    - Adding unconverted entries
      - For example, LR flag of Breakup interaction
  - Class package
    - Reduce memory consumption
- Cooperation with other models
  - Currently as much as follows the description of G4NDL (ENDF) , but is this good idea?

# Thermal neutron scattering from chemically bound atoms

- At thermal neutron energies, atomic translational motion as well as vibration and rotation of the chemically bound atoms affect the neutron scattering cross section and the energy and angular distribution of secondary neutrons.
- The energy loss or gain of incident neutrons can be different from interactions with nuclei in unbound atoms.

# Thermal neutron scattering files from the evaluated nuclear data files ENDF/B-VI, Release2

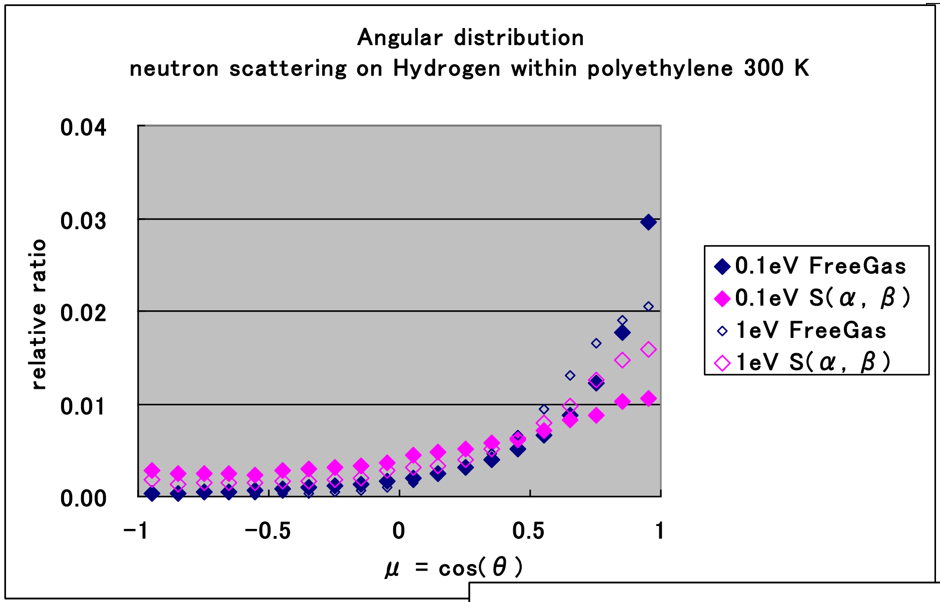
- These files constitute a thermal sub-library
- Use the File 7 format of ENDF/B-VI
- Divides the thermal scattering into different parts:
  - Coherent and incoherent elastic; no energy change
  - Inelastic; loss or gain in the outgoing neutron energy
- The files and NJOY are required to prepare the scattering law S(α,β) and related quantities.

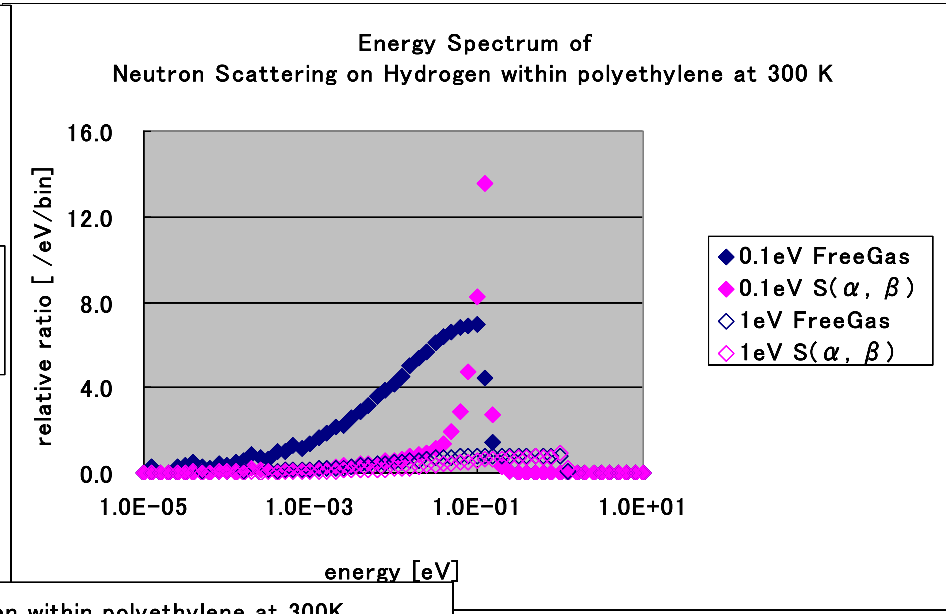
$$\text{Scattering cross section: } \sigma(E \rightarrow E', \mu) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}S(\alpha, \beta);$$

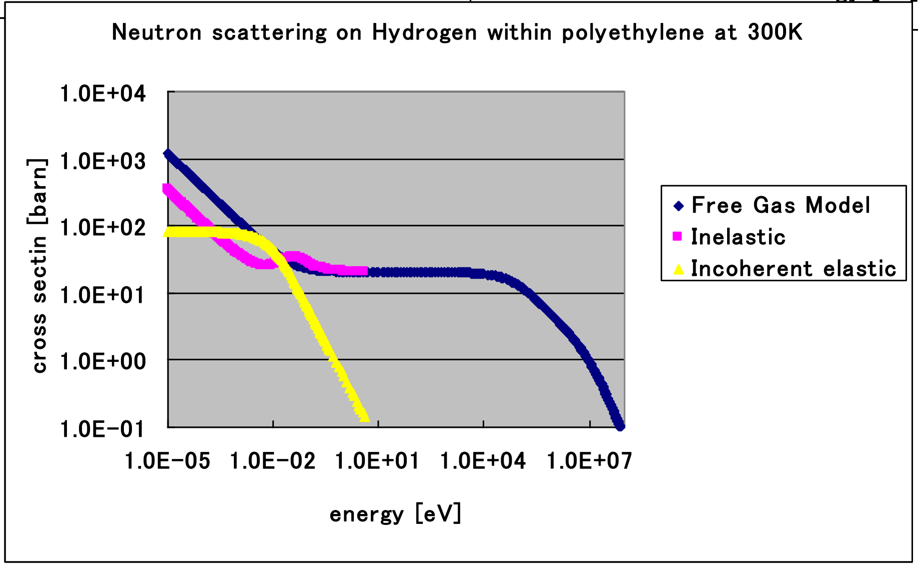
$$\text{momentum transfer: } \alpha = \frac{E' + E - 2\sqrt{E'E}\mu}{AkT}, \text{ energy transfer: } \beta = \frac{E' - E}{kT}$$

Comparison of
cross sections and final states
between free gas model and
thermal scattering model S(α,β)

# Cross section and Secondary Neutron Distributions using S(α, β) model



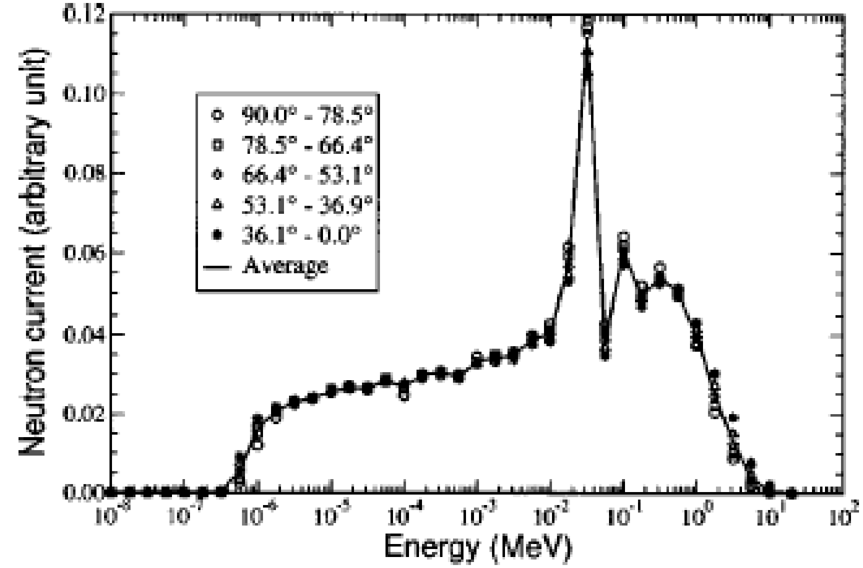



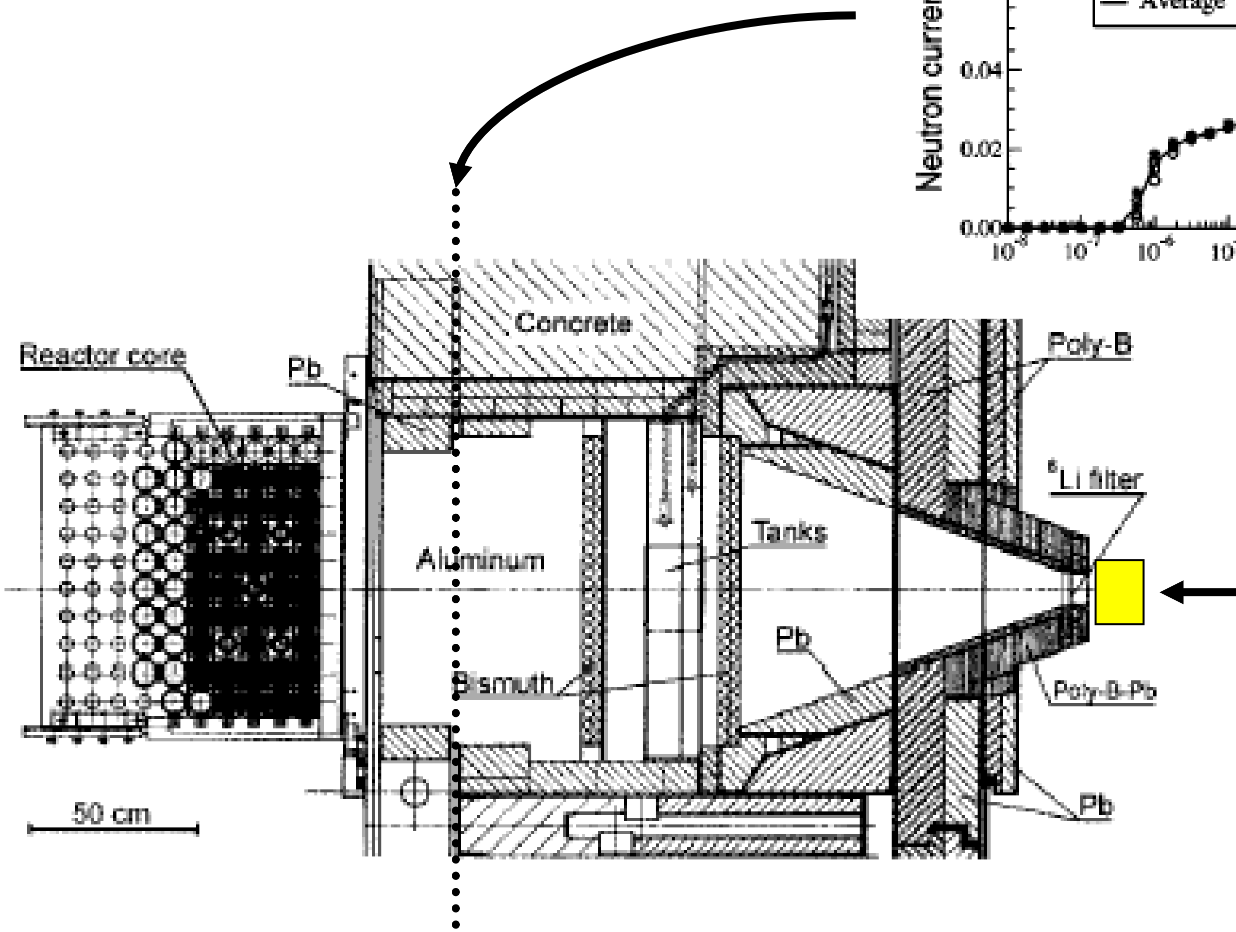
# Validation with measurements

The neutron capture therapy (NCT) facility at the Studsvik, Sweden.

# The NCT facility at the Studsvik, Sweden

Calculated neutron energy spectra



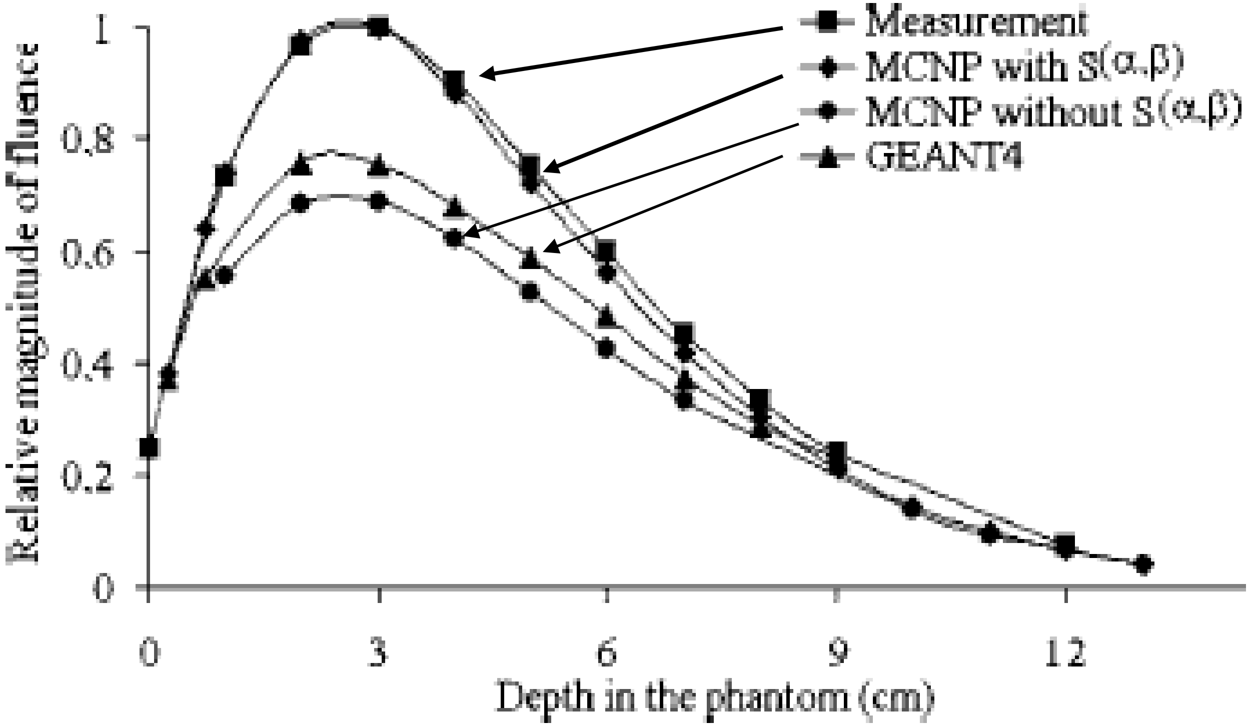




PMMA Phantom
20x20x15 cm$^3$

Horizontal cross-sectional view of the Studsvik R2-0 reactor and the BNCT clinical beam.

**Giusti et al.,**
**Med. Phys. (30) 3107 (2003),**

# Enger *et al.*, Med. Phys. (33) 337 2006




In this paper they said that "The location of the thermal neutron peak calculated with MCNP without *S(α,β)* , and GEANT4 is

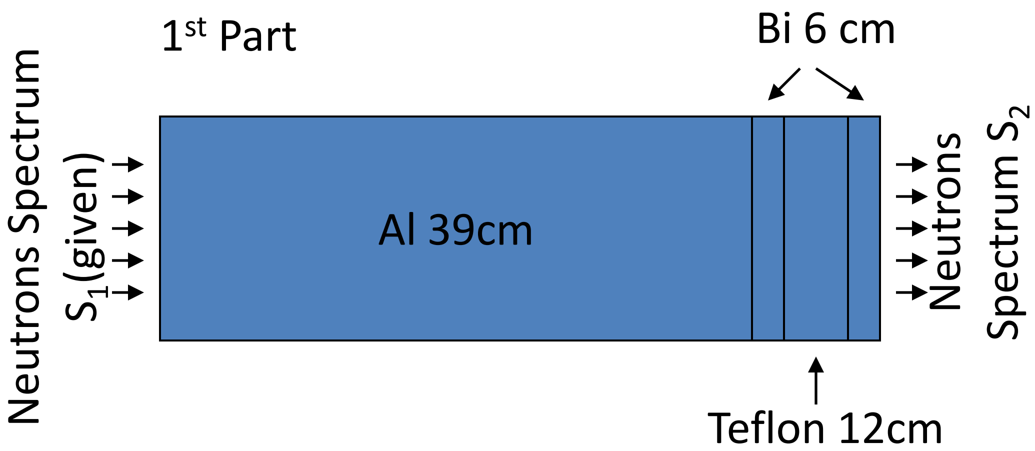
shifted by about 0.5 cm towards a shallower depth and is

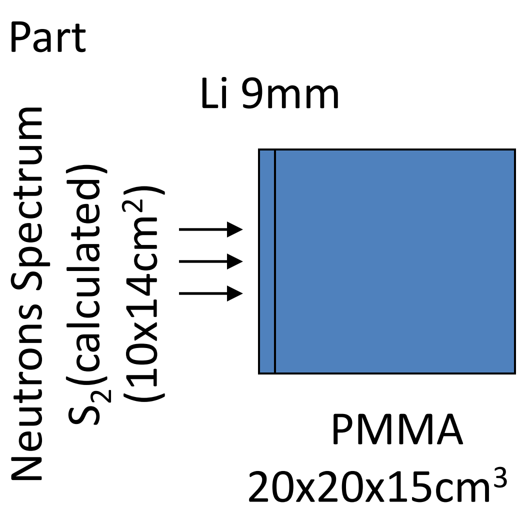
25%–30% lower in amplitude."

FIG. 2. Relative thermal neutron fluence. The MCNP calculation with $S(\alpha,\beta)$ is normalized to the measurement on the beam centerline at the reference point of 3 cm. The GEANT4 and MCNP calculation without $S(\alpha,\beta)$ are also normalized at the reference point to the MCNP results that are normalized to the measurement.

# Geant4 simulation for BNCT clinical beam simulation is divided into two part

- 1st : Slowing down fast neutrons
  - Start from given neutron spectrum $S_1$
  - Aluminum (39cm)
    + Bismuth (6cm)
    + Teflon (12cm)
    + Bismuth (6cm)
  - Get Neutron spectrum after these materials $S_2$
- 2nd :Transportation in the phantom
  - Start from $S_2$
  - Li filter (9mm)
    + PMMA (20x20x15 $cm^3$)
  - Get neutron fluencies in the phantom
  - Thermal scattering of Hydrogen within Polyethylene is used for H in the PMMA



# Results

# with previous measurement and calculations

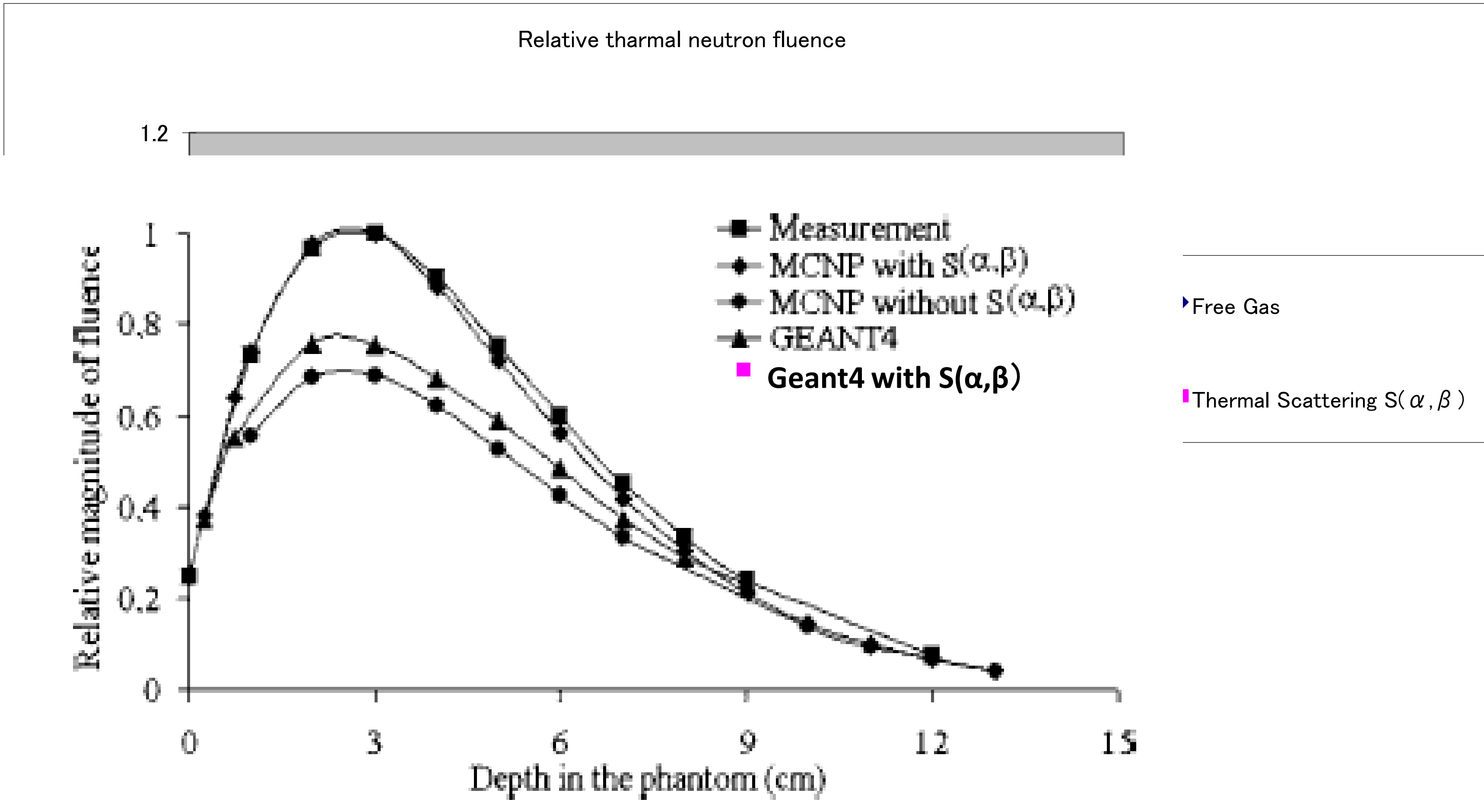



FIG. 2. Relative thermal neutron fluence. The MCNP calculation with $S(\alpha,\beta)$ is normalized to the measurement on the beam centerline at the reference point of 3 cm. The GEANT4 and MCNP calculation without $S(\alpha,\beta)$ are also

# Issues for Thermal Scattering

- Usage is slightly difficult
  - User must define (G4)material by (G4)element with specific names like “TS_H_of_Water”.
  - Cannot access to “material” from hadronic XS.
  - Better idea?
- Currently only 3 elements data are converted
  - H_of_Water, H_of_Plolyethelen and Graphite
  - ENDF/B-VII Thermal Data provides 20 elements
  - We may need to migration effort to ENDF/B-VII
  - MCNP has more data than ENDF(?) (For example Sappier)

# Issues for G4NDL and NeutronHP (1)

- Checking completeness of supported FORMAT
  - All FORMAT which are used in the recent libraries (ENDF-VII, JEND4.0, JEF3.1 and so on) is supported or not?
  - FOMAT means set of “LTT, LCT, LI, LF, LAW and so on in MFs.
  - Does someone created FULL list of
    - Which FORMAT is supported or not in NeutornHP
    - Which FORMAT is used in the recent libraries

# Issues for G4NDL and NeutronHP (2)

- Re-design both data format and package classes
  - Data Format
    - Enable to use temperature specified data
      - Want to this shortly
    - Adding unconverted entries
      - For example, LR flag of Breakup interaction
  - Class package
    - Reduce memory consumption
      - Timing of building physics table
        - » Building only necessary data
    - Better physics performance
      - Conservations and distribution
    - Better maintainability

# Issues for G4NDL and NeutronHP (3)

- Cooperation with other Geant4 models
  - Currently as much as follows the description of G4NDL (ENDF)
  - But is this good idea?
  - We may push cooperation with other Geant4 models, especially in final state generation