The low energy neutron (particle) project of LLNL/SLAC G4LEND-GIDI

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Low energy nuclear data

- Nuclear data for reaction of projectile hitting a target
  - Example: n + 16O ⇒ n + p + 15N
- Most data are
  - For neutron as projectile
  - Low projectile energies: 10E-11 to 20 MeV
- In legacy formats
  - ENDL (Evaluated Nuclear Data Library)
    - Developed at LLNL ~1960
  - ENDF (Evaluated Nuclear Data File)
    - Developed by international committee ~1964

Issues with legacy formats

- Have a fixed number of supported reactions
  - The following reaction is not support

    n + 79Kr ⇒ 2H + n + 3H + 74Se
  - Fixed precision format
- Very difficult to read – try reading ENDF formatted data
- Format does not represent physics
- New format and infrastructure are designed to solve many issues

No more punch cards

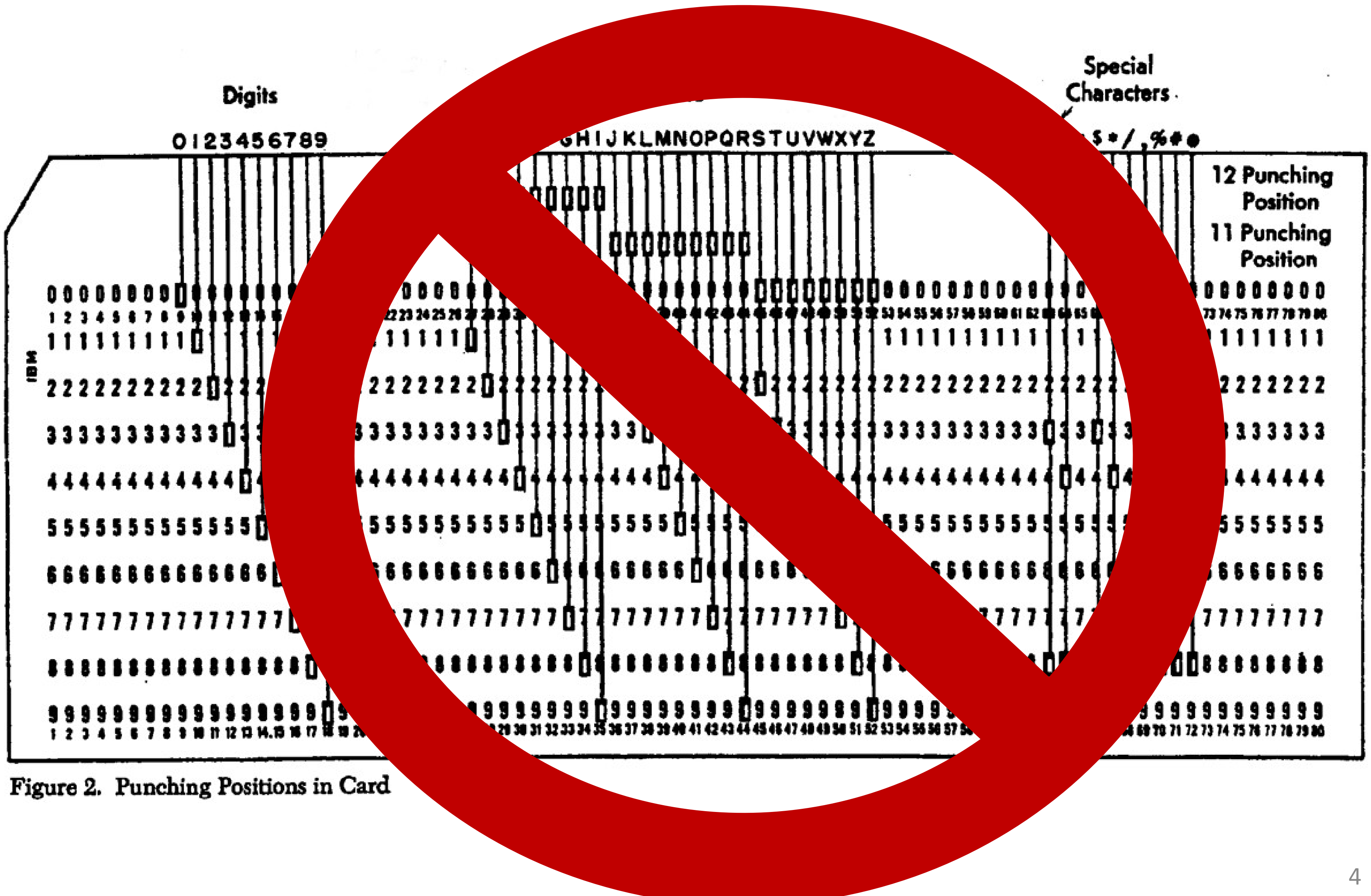


Figure 2. Punching Positions in Card

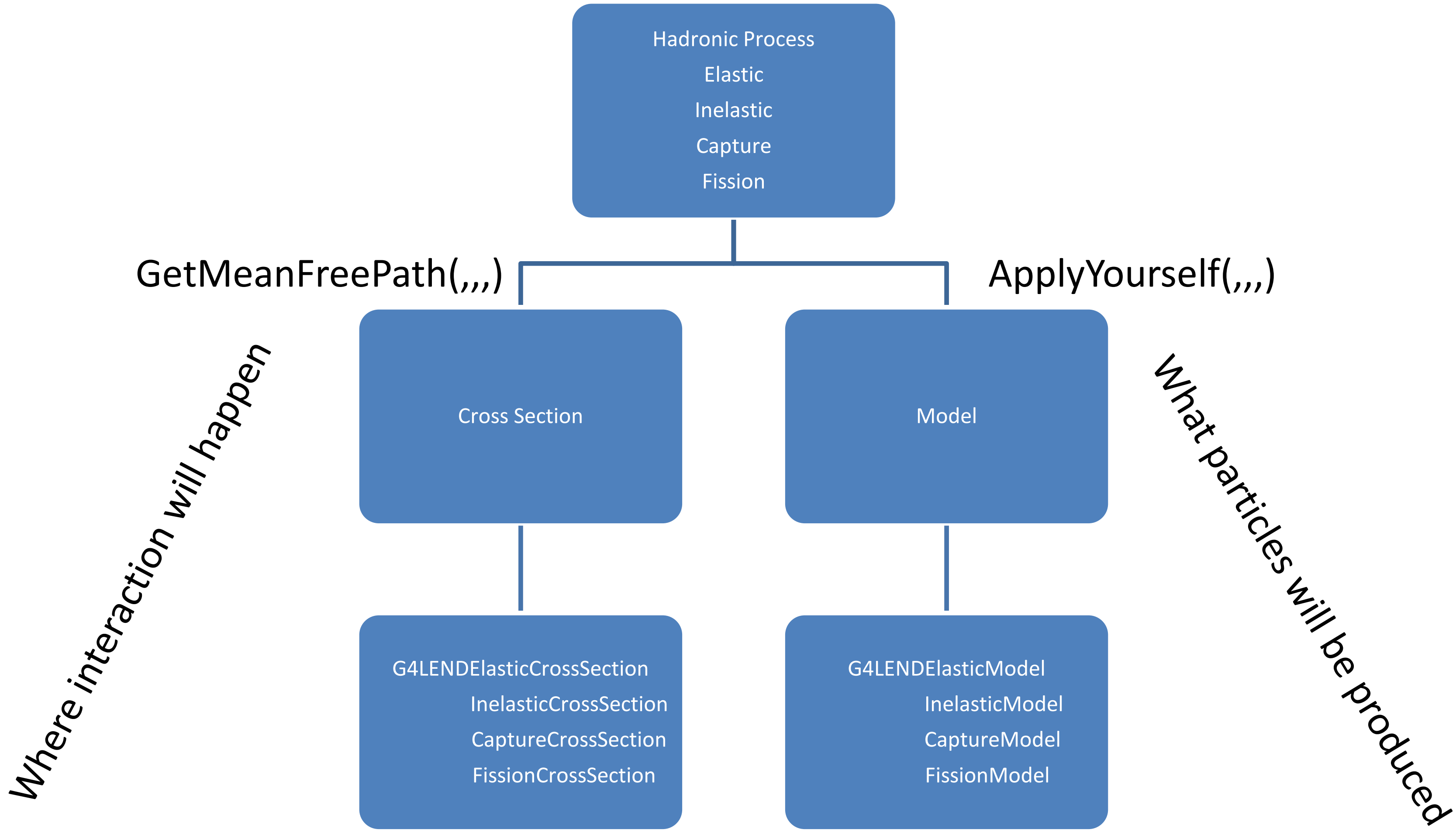
General Interaction Data Interface (GIDI) and Geant4 Low Energy Nuclear Data (G4LEND)

- GIDI is a newly developed data format for nuclear data
  - More modern design than current nuclear formats established in the 1960'
- GIDI also provide access routines for the data
- Conversion of the current nuclear data bases such as ENDF(USA), JEFF(Europe), JENDL(Japan), ENDL(LLNL) are on going
- LEND is Geant4 interface for GIDI

G4LEND

- Geant4 interface to GIDI
- Follows Hadronic Framework of Geant4, separated cross section and model as final state generator
- Manage target nuclei data in GIDI
- Pre-calculated data for certain temperatures are used.
  - 300, 1160 and 3590 K
- An alternative to the low energy neutron package (NeutronHP) in Geant4

Geant4 Hadronic Framework



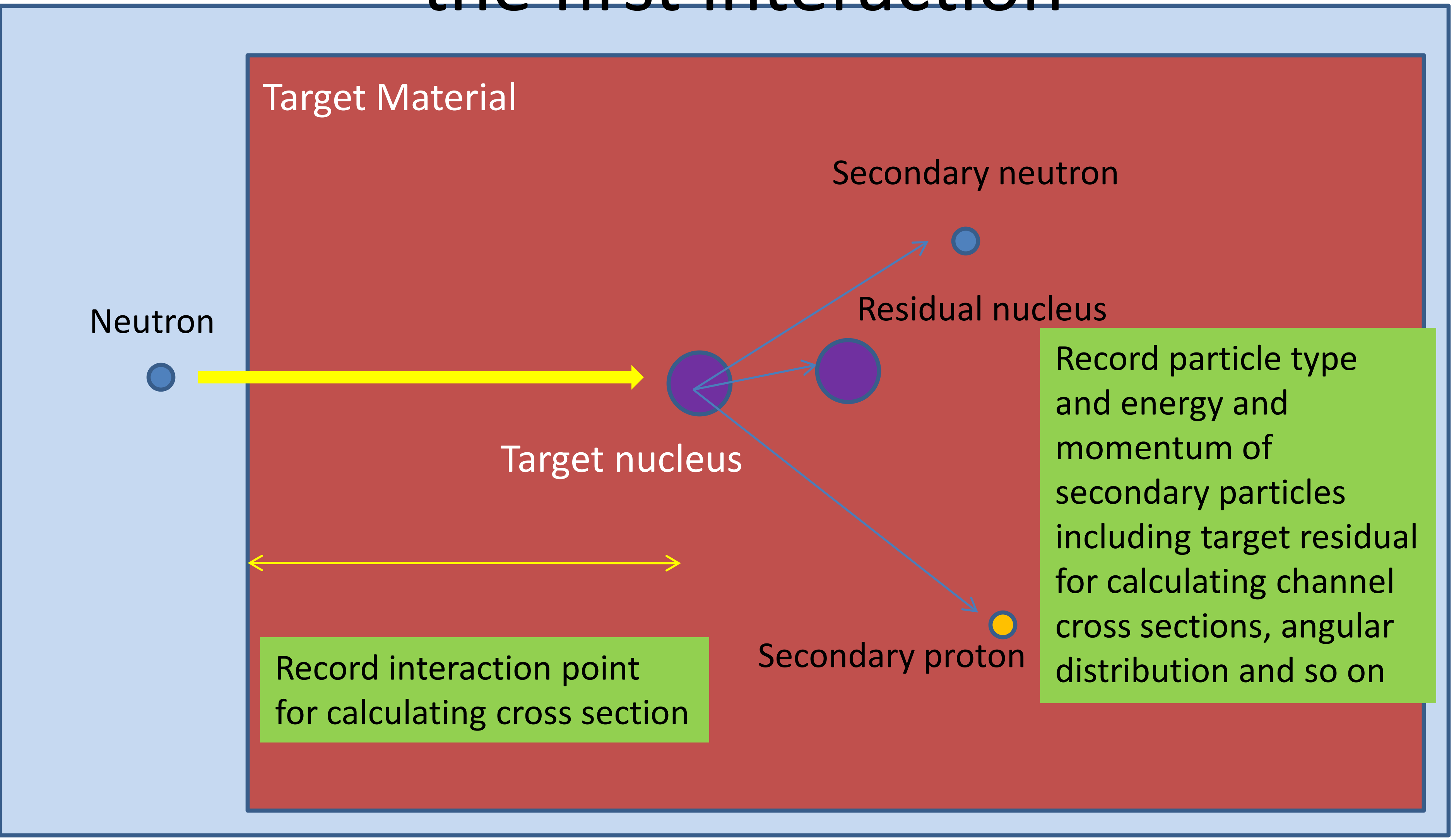
ENDL99

- ENDL99 is the nuclear database used at LLNL for long time.
- 109 isotopes data from H to Cf, including 27 natural abundance element
  - See next slide for full list
  - Total size 240MB in xml format. (unzipped)
- Select as the first dataset converted to the GIDI format
- The original converter to new nuclear format does not written ENDF format.
- Energy range
  - From 20MeV down to thermal energy (10E-4)

Full list of target isotope (element) of ENDL99

n_1
H_1
H_2
H_3
He_3
He_4
Li_6
Li_7
Be_7
Be_9
B_10
B_11
C_12
C_13
N_14
N_15
O_16
F_19
Ne_20
Na_23
Mg_natural
Al_27
Si_natural
P_31
S_32
Cl_natural
Ar_natural
K_natural
Ca_natural
Ti_natural
V_51
Cr_natural
Mn_55
Fe_natural
Co_59
Ni_58
Ni_natural
Cu_natural
Zn_natural
Ga_natural
As_74
As_75
Y_88
Y_89
Zr_natural
Nb_93
Mo_natural
Ag_107
Ag_109
Cd_natural
In_natural
Sn_natural
Sb_natural
I_127
Xe_134
Xe_natural
Ba_138
Eu_natural
Gd_natural
Ho_165
Hf_natural
Ta_181
W_natural
Re_185
Re_187
Pt_natural
Au_197
Hg_natural
Pb_natural
Bi_209
Th_231
Th_232
Th_233
Pa_233
U_233
U_234
U_235
U_236
U_237
U_238
U_239
U_240
Np_235
Np_236
Np_237
Np_238
Np_237
Np_238
Pu_237
Pu_238
Pu_239
Pu_240
Pu_241
Pu_242
Pu_243
Am_241
Am_242_m
Am_243
Cm_242
Cm_243
Cm_244
Cm_245
Cm_246
Cm_247
Cm_248
Bk_249
Cf_249
Cf_250
Cf_251
Cf_252

Simulation in material up to the first interaction

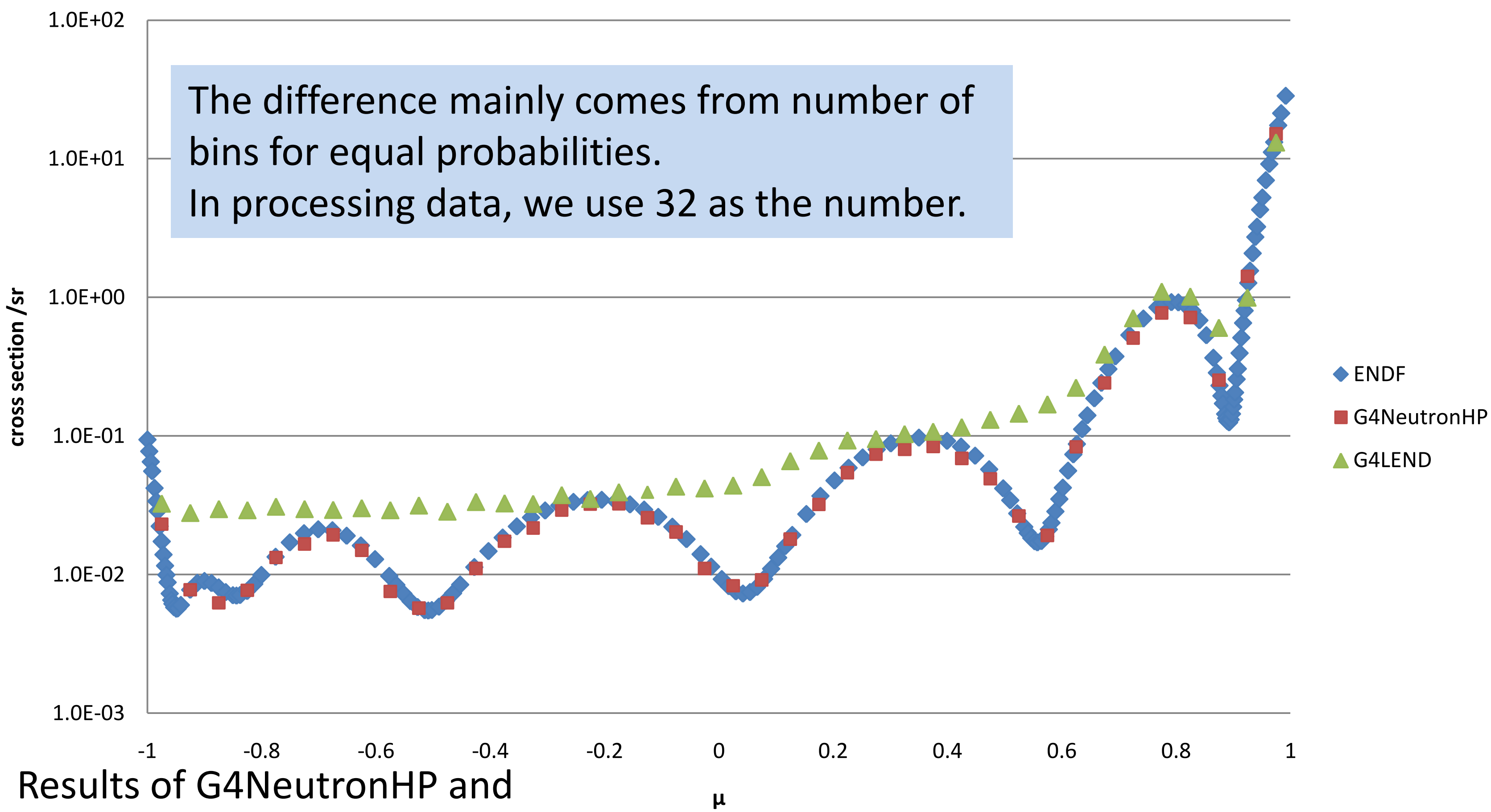


Channel Cross Section
n (16MeV) on Au

	ENDF VII	G4NeutornHP	G4LEND
Total	5.468 [barn]	5.40	5.41
Elastic	2.785	2.74	2.86
Capture	5.56e-4	9.1e-4	96.e-4
Inelastic			
(n,2n)	2.232	2.21	2.10
(n,3n)	2.75e-2	2.7e-2	2.9e-2
(n,p)	3.60e-3	3.1e-3	5.4e-3
(n,a)	1.00e-3	0.9e-3	1.4e-3

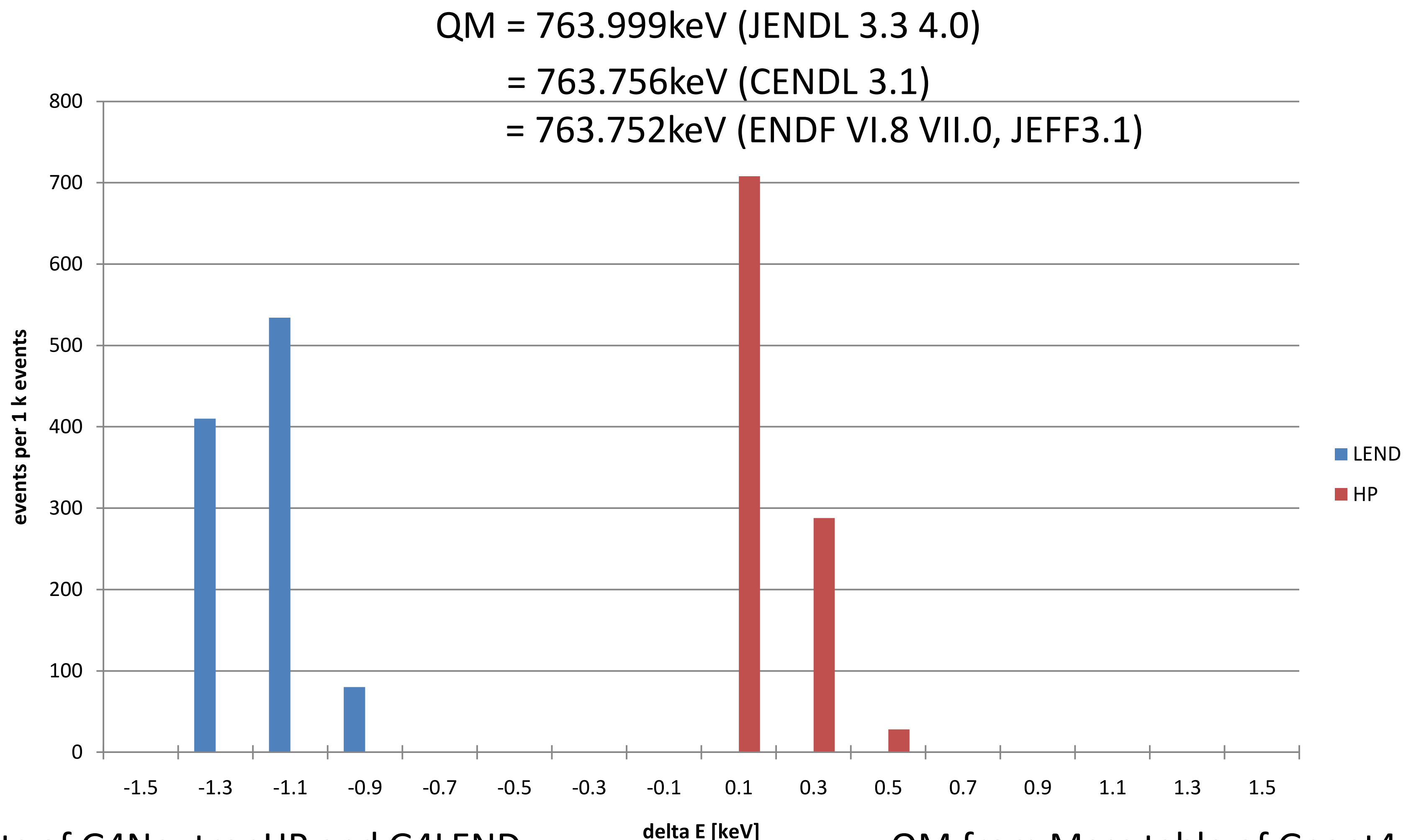
Results of G4NeutronHP and G4LEND are derived by a thin target like simulation

Angular Distribution of neutrons n (16MeV) on Au



Results of G4NeutronHP and G4LEND are derived by thin target like simulation

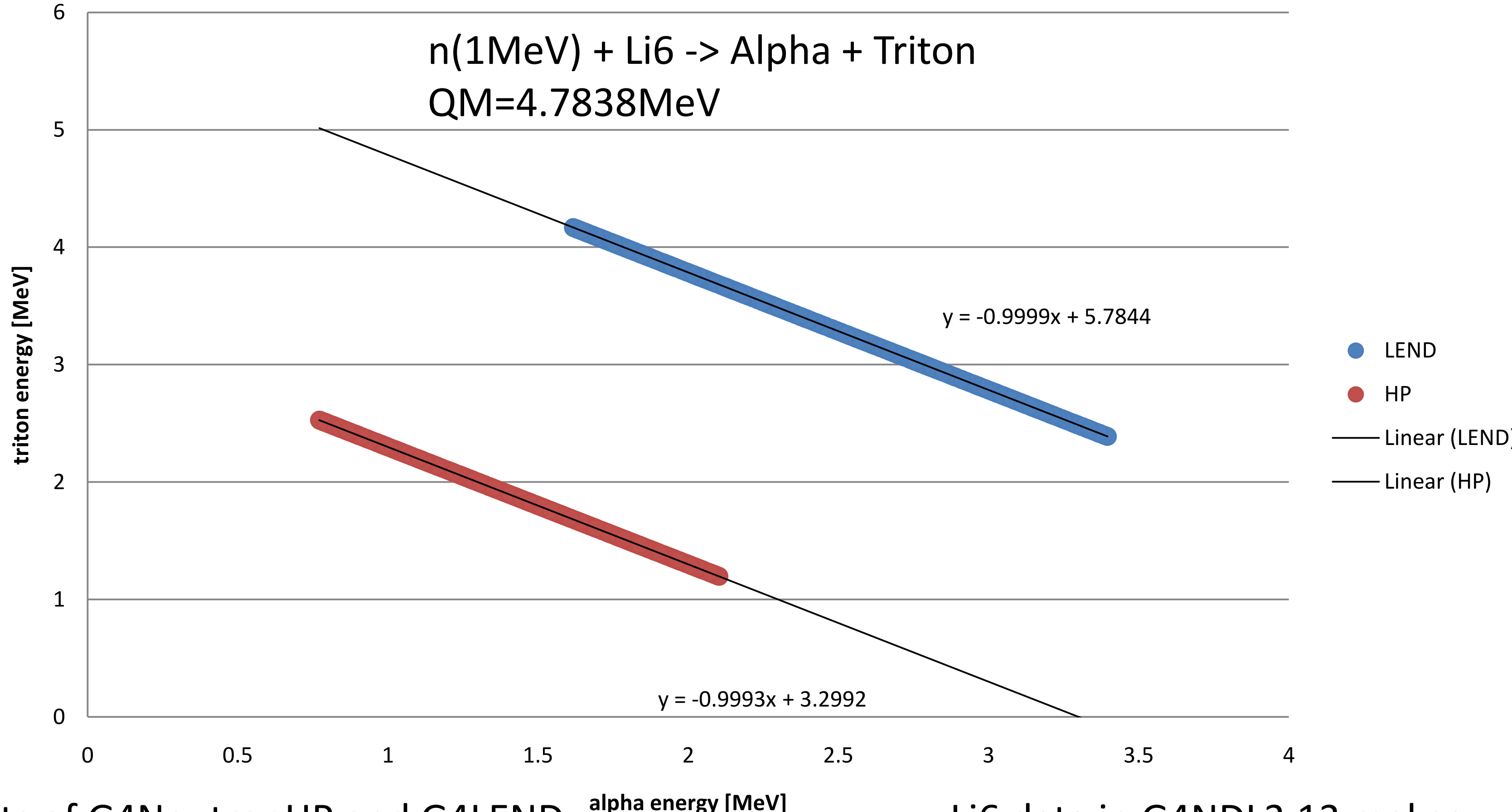
Level of energy conservation n(1MeV) + 3He → 3H + 1H



Results of G4NeutronHP and G4LEND are derived by thin target simulation

QM from Mass table of Geant4 (AEM03 and PDG) = 763.347keV

Example of problem fixed in G4NDL(v9.4)

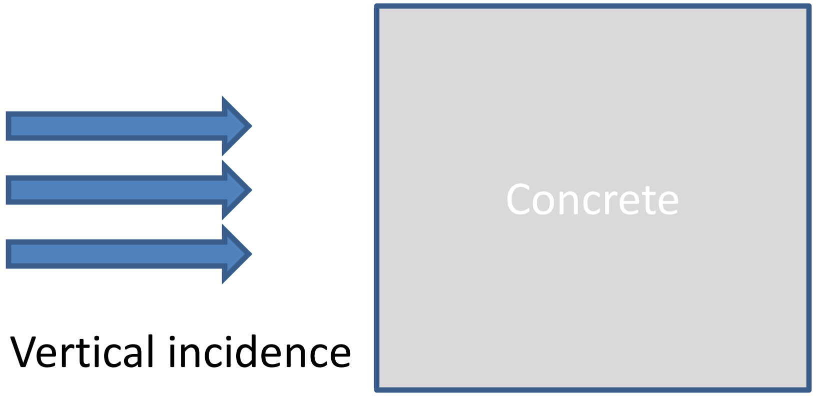


Results of G4NeutronHP and G4LEND are derived by thin target simulation

Li6 data in G4NDL3.13 makes this trouble, and the data will be updated in the next version

Neutron Attenuation in Iron and Concrete Slab

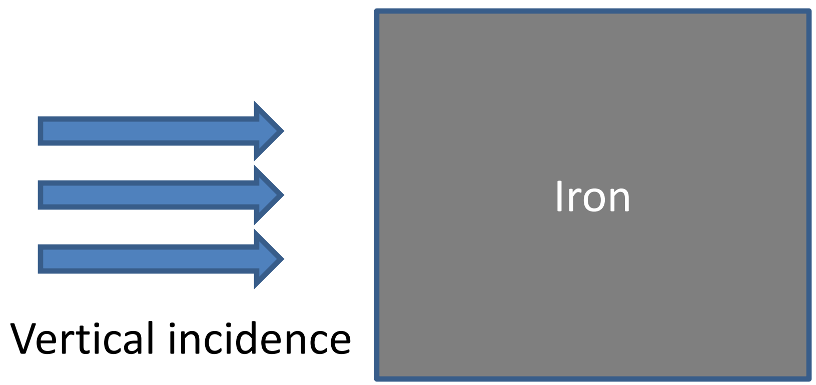
neutrons
uniformly distributed
within 45-50MeV



Concrete
Density 2.27 g/cm^3

Element	Weight percent
H	1.02
C	0.10
O	53.85
Mg	0.22
Al	3.44
Si	34.22
K	1.32
Ca	4.41
Fe	1.41

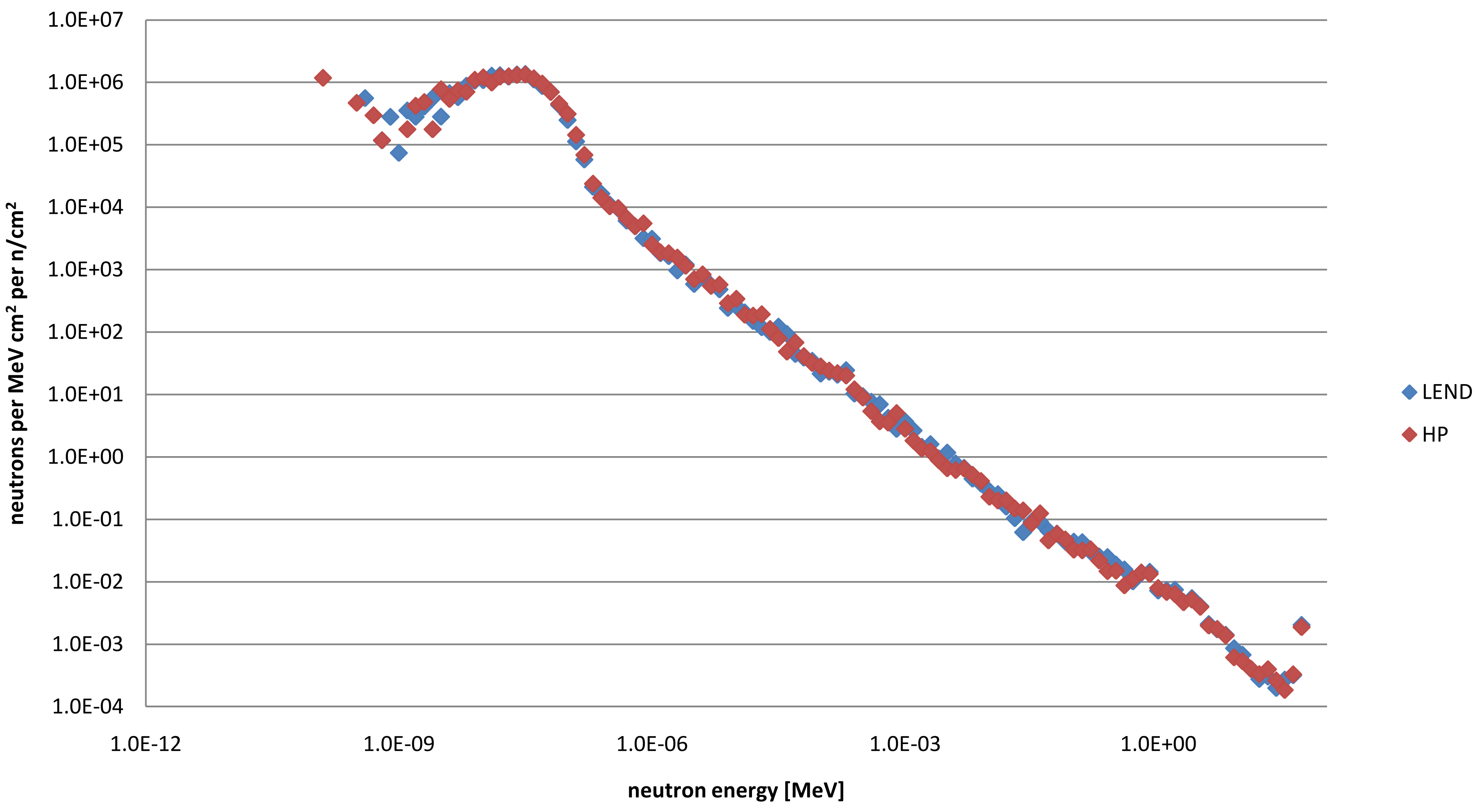
neutrons
uniformly distributed
within 45-50MeV



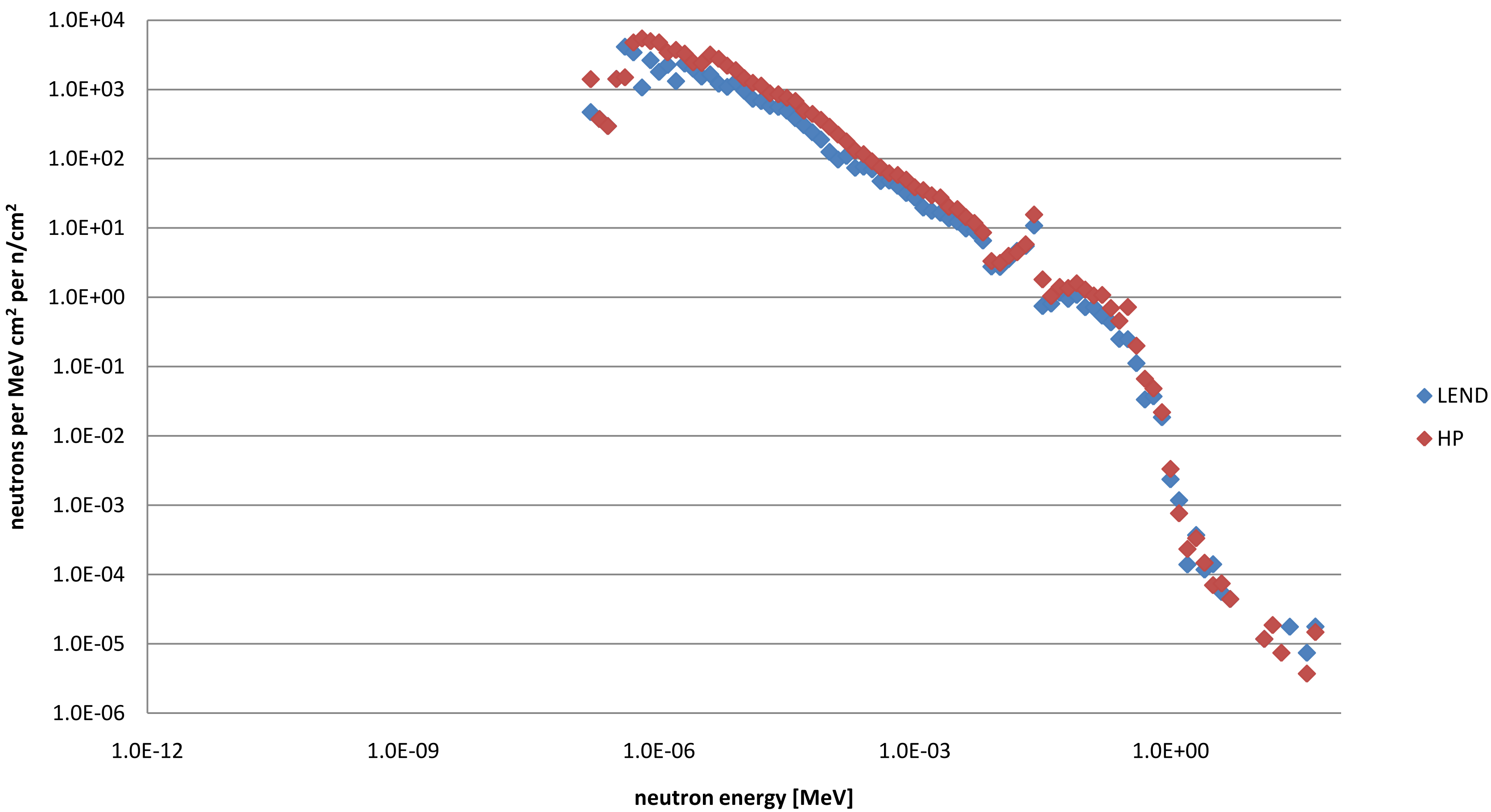
Iron
Density 7.87 g/cm^3

First and some secondaries interactions of primary neutrons are calculated by Geant4 Bertini model

45-50MeV neutrons bombarding concrete slab Neutron energy spectrum at depth of 1m



45-50MeV neutrons bombarding Iron slab Neutron energy spectrum at depth of 1m



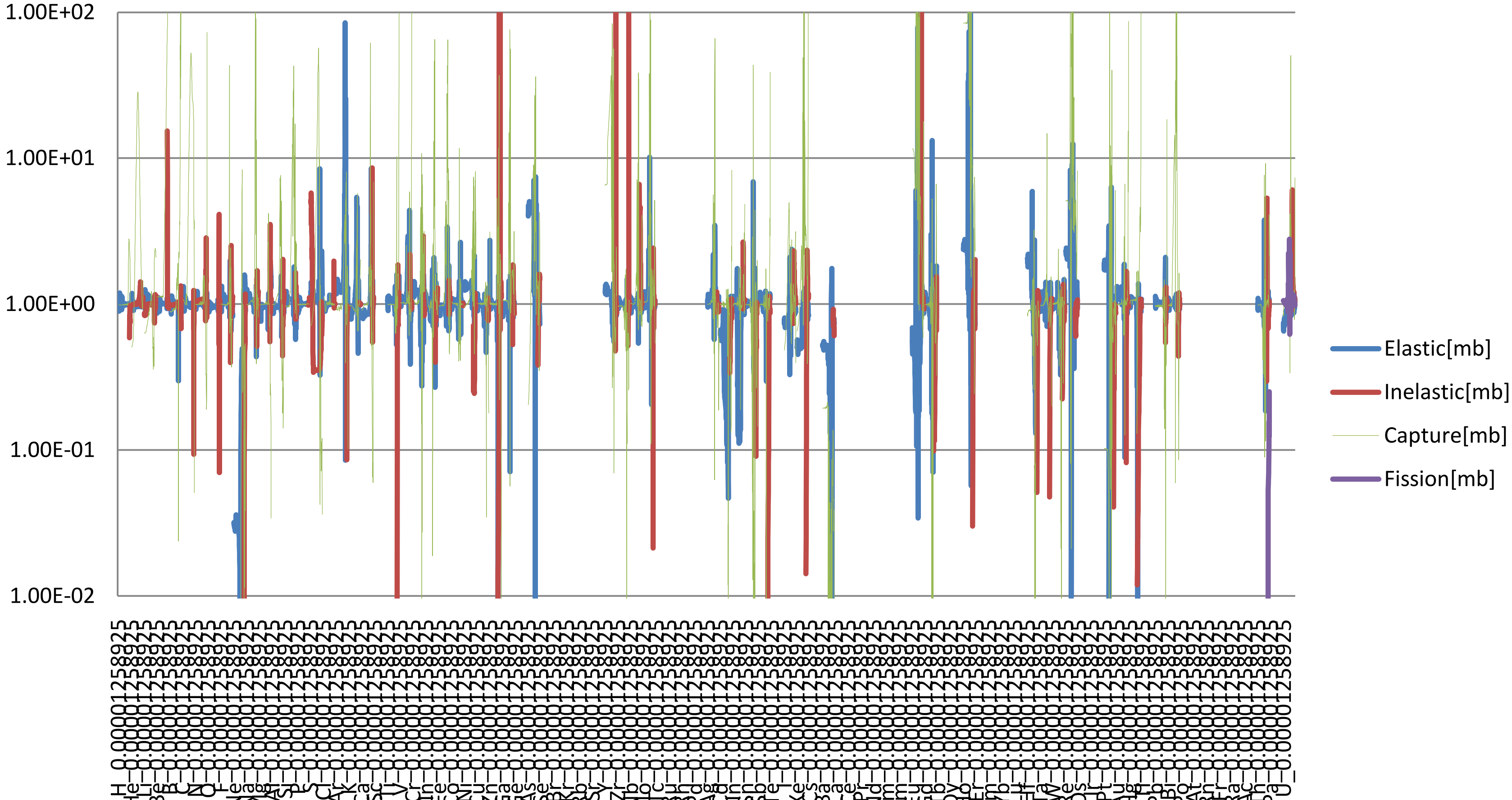
QGSP_BERT_LEND Physics List

- A proposed reference physics list which uses LEND (neutron) instead of NeutronHP
- “QGSP_BERT_LEND”
  - G4NeutronLENDBuilder
  - G4HadronElasticPhysicsLEND
  - HadronPhysicsQGSP_BERT_LEND
- Neutron time cut (10(?) micro sec)

Elemental Cross Section Check

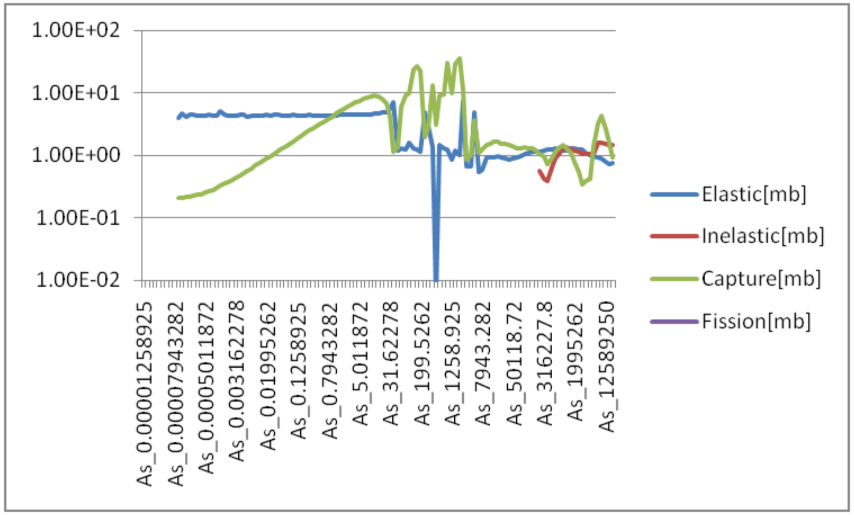
- Create G4_H to G4_U
- Configure PhysicsList
- Compare (Partial) Cross Section by
  - PROCESS->GetMicroscopicCrossSection(,,,)”
- This value is really Geant4 used in a simulation.

Checking cross section ratio HP/LEND from H to U

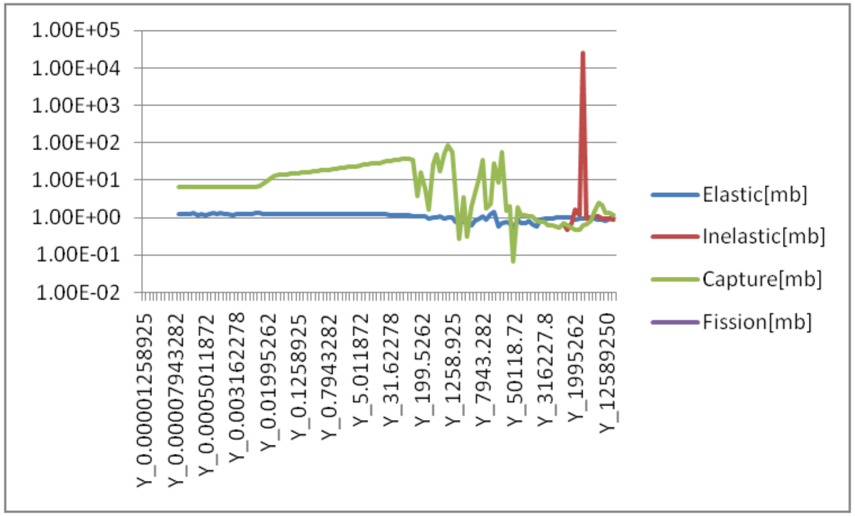


Close-up to interested element

As 75

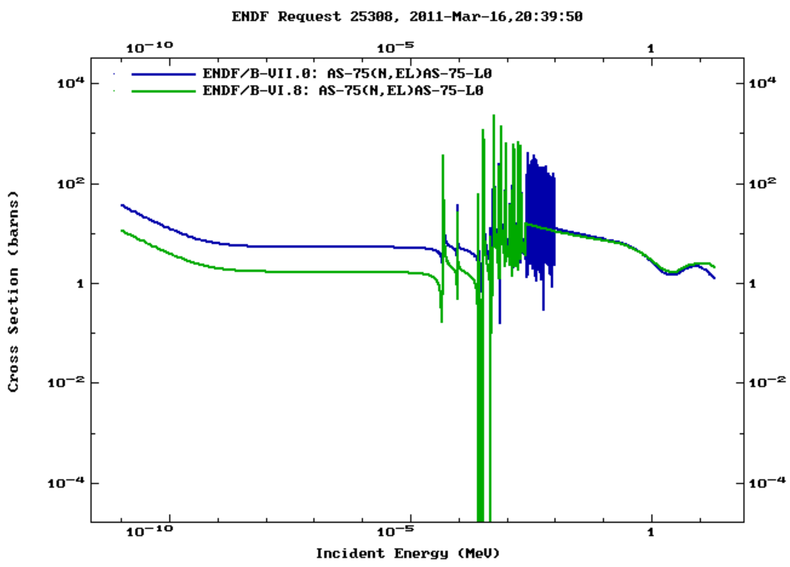


Y 89



Difference in ENDF VI and VII of the elements

As 75



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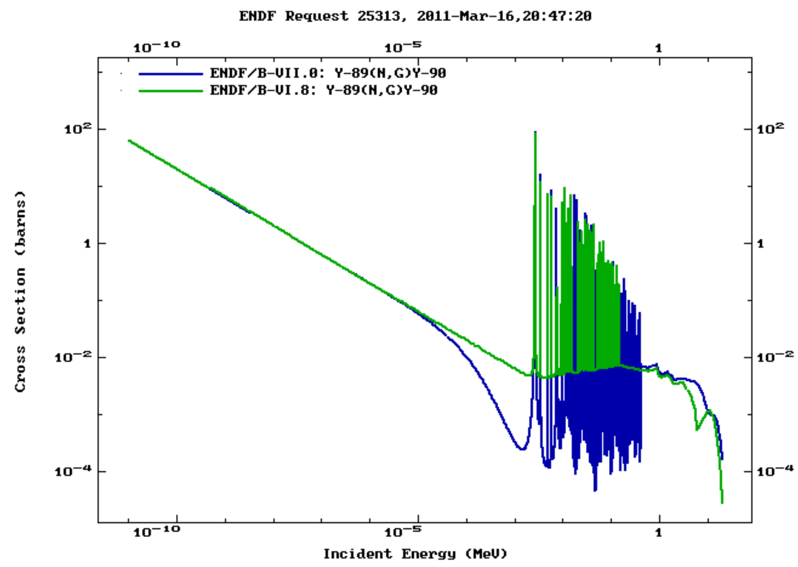


ATLAS Cavern Background Simulation

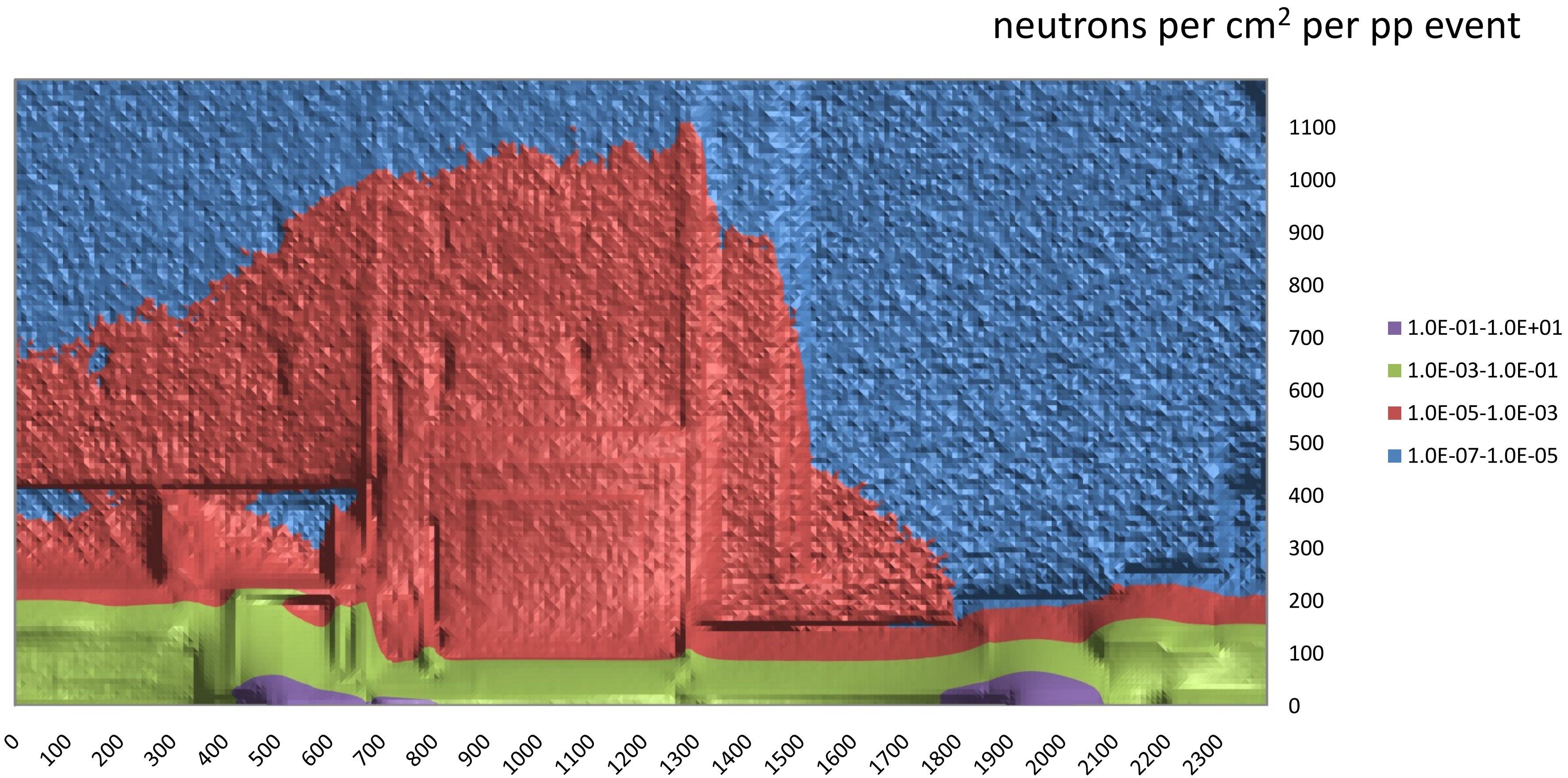
- Physics List “QGSP_BERT_LEND”
- Geometry “Atlas Cavern Background Simulation”
- “ENDL99” has at least “natural element data” for the materials in the simulation

Comparison of CPU and Memory Consumption

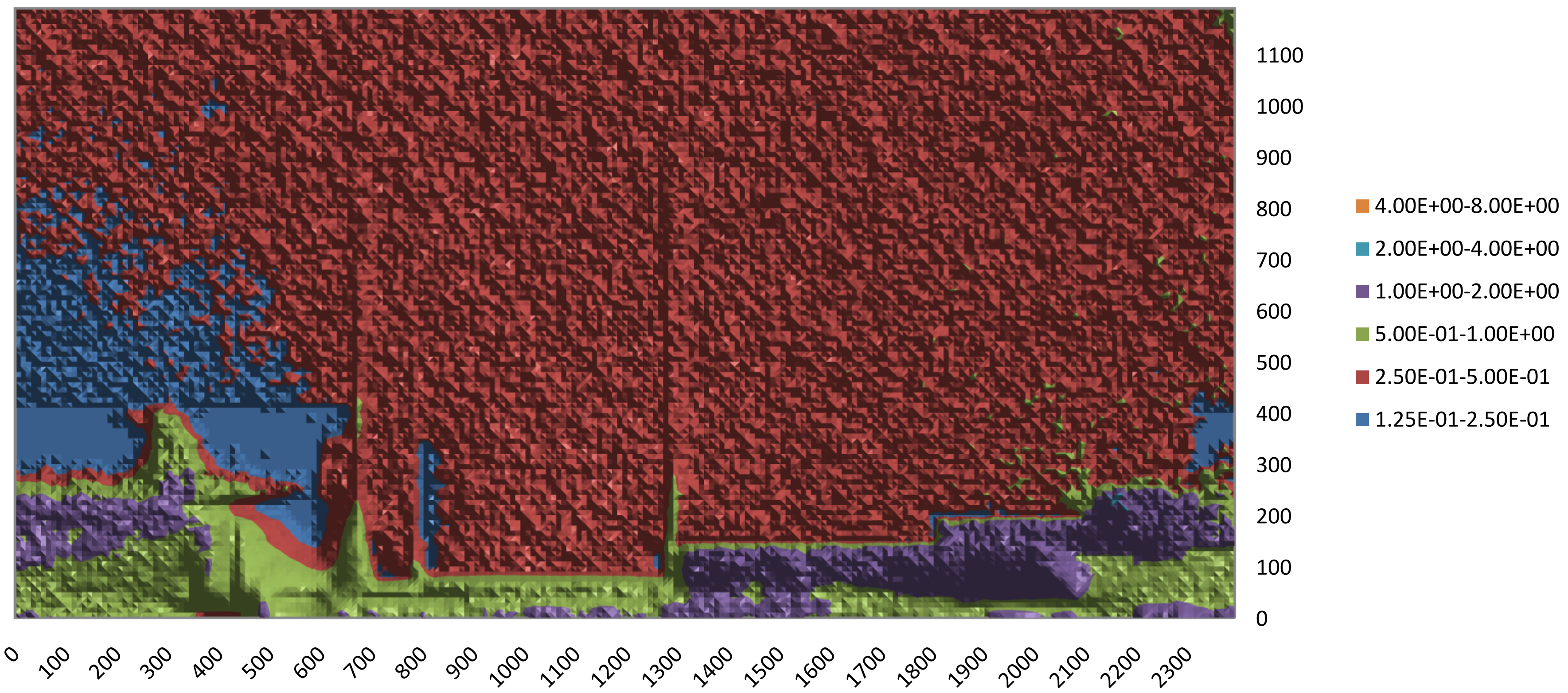
based on ATLAS Cavern Background 64 7TeV pp events

- 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_LEND
  - 300 sec/event, 160MB

QGSP_BERT_LEND
neutorn



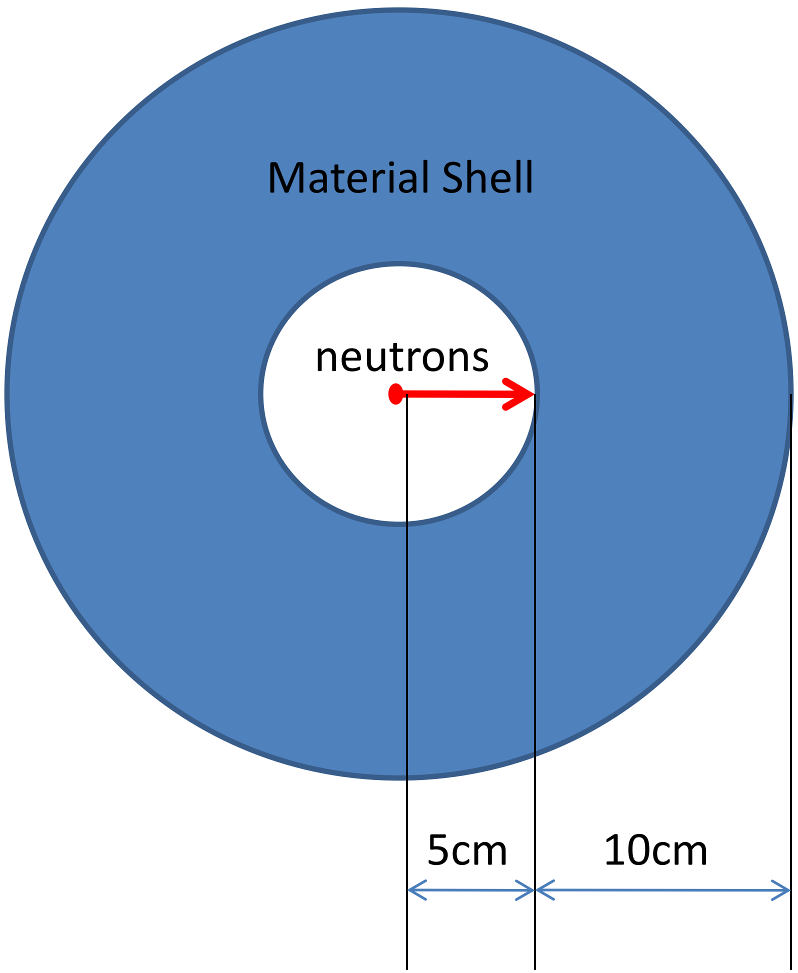
QGSP_BERT_HP/QGSP_BERT_LEND
neutorn



GAMOS comparison

- Requested by Pedro
- Neutron energy spectrum after certain amount (10cm) of materials
- His main interest is shape and position of thermal peak.
  - In some case there are relatively large deference to MCNP result

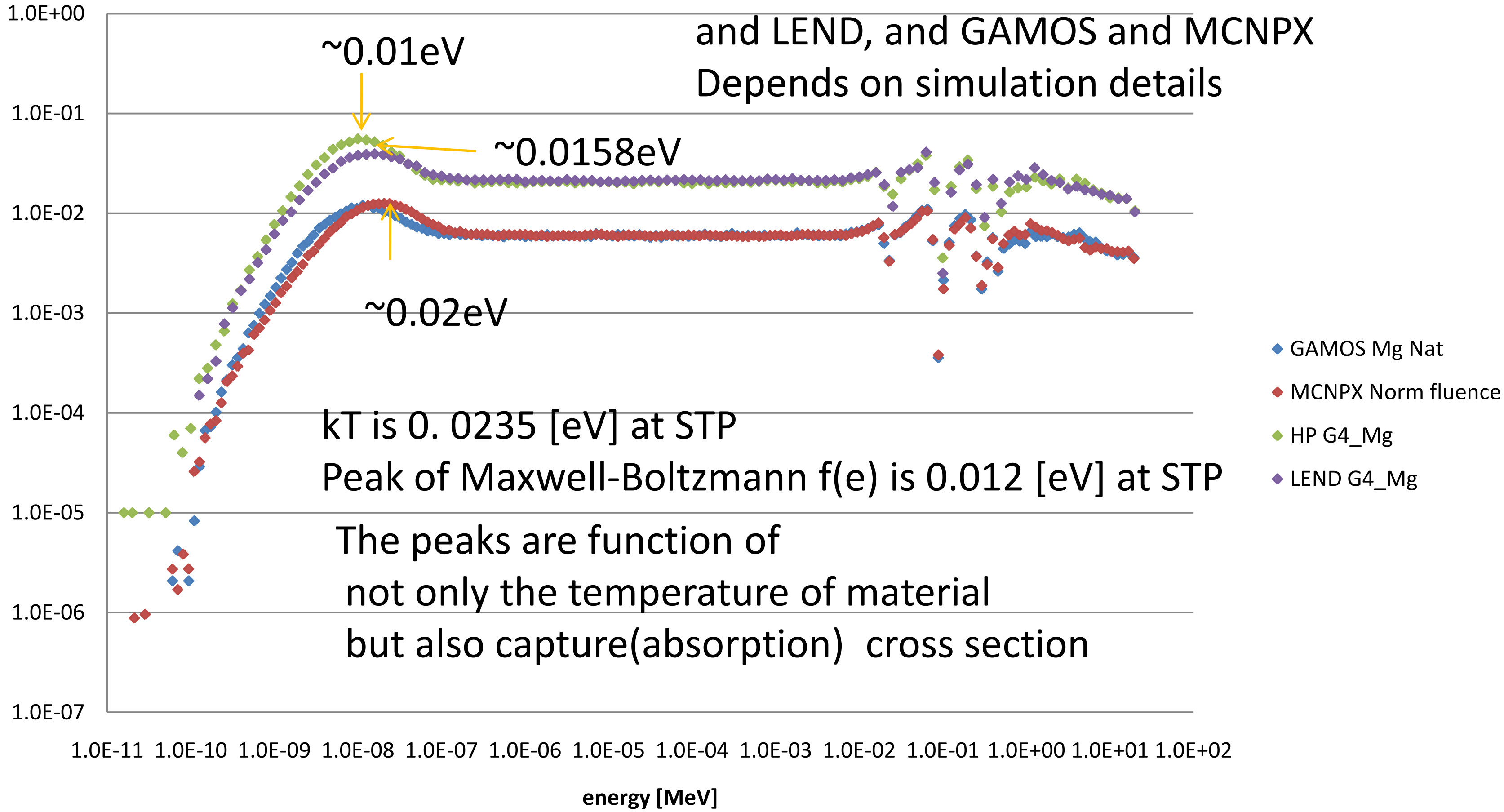
Condition of GAMOS comparison



- 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

An example of GAMOS comparison

Different normalization used between HP and LEND, and GAMOS and MCNPX
Depends on simulation details



Same kind of plots are available for
O16 O17 Na23 Mg_nat Al27 Si28 Si29 Si30 Cl35 Cl37 K_nat
Ca_nat Fe54 Fe56 Fe57 Mn55 Pb204 Pb206 Pb207 and Pb208

How to use LEND and QGSP_BERT_LEND

- LEND and its ENDL99 is already in Geant4 repository
- Checkout trunk of "source/processes/hadronic/models/lend"
- Edit GNUmakefile"source/processes/hadronic/models"
  - Add

    SUBDIRS += lend
    SUBLIBS += G4had_lend

  at proper positions.

  You may need update of "libname.map".
- Set environment variable of "G4LENDDATA"
- Edit GNUmakefile of you application
  - Add

    CPPFLAGS += -I$(G4INSTALL)/source/processes/hadronic/models/lend/include
    EXTRALIBS += -lexpat
    at proper positions

How to build and use LEND and QGSP_BERT_LEND (cont.)

- "QGSP_BERT_HP" is not yet in the repository.
  - Cause compile errors for who does not check out "LEND".
- Please allow tar ball based distribution for a while.
- Unpack the tar ball at "source/physics_lists" and make.
  - You may need "make clean" at first.
- Include "QGSP_BERT_LEND.hh" in your application.
  - You cannot use the physics list through "PhysicsListFacotry"

Typical Physics List for LEND

```
#include "G4HadronElasticProcess.hh"
#include "G4LENDElasticCrossSection.hh"
#include "G4LENDElastic.hh"

*********************************************************************************
// “particle” is the particle definition of neutron (G4Neutron)
// “pmager” is the process manger of neutron (G4Neutron)

G4HadronElasticProcess* theNeutronElasticProcess = new G4HadronElasticProcess();

//setup LEND XS and model

G4LENDElasticCrossSection* endlElasticXS = new G4LENDElasticCrossSection( particle );
endlElasticXS->AllowNaturalAbundanceTarget();
//endlElasticXS->AllowAnyCandidateTarget();
G4LENDElastic* endlElasticFS = new G4LENDElastic( particle );
endlElasticFS->AllowNaturalAbundanceTarget();
//endlElasticFS->AllowAnyCandidateTarget();
theNeutronElasticProcess->AddDataSet( endlElasticXS );
theNeutronElasticProcess->RegisterMe( endlElasticFS );
pmanager->AddDiscreteProcess( theNeutronElasticProcess );
```

GIDI ver2

- We are already working for LEND-GIDI ver2.
- At this version, we will convert not only ENDL(LLNL) but also most of nuclear data libraries (ENDF(USA), JEFF(Europe), JENDL(Japan),CENDL(Chaina) ROSFOND(Russia) to the GIDI format.

Summary

- We are developing G4LEND which is Geant4 interface for the GIDI.
- This will be an alternative choice of low energy neutron transportation in Geant4
- First comparison against ENDF data and Neutron HP has reasonable agreement
- Plan is to include G4LEND in the next Geant4 beta release (June,2011)
- GIDI library and data should also to be available at that time
  - They will be separately distributed from Geant4